ATOM 1 N GLY A 1120.138 11.140 -2.903 1.00 0.00 N ATOM 2 CA GLY A 1120.658 10.305 -1.785 1.00 0.00 C ATOM 3 C GLY A 1120.202 8.862 -1.879 1.00 0.00 C ATOM 4 O GLY A 1119.025 8.590 -2.119 1.00 0.00 O ATOM 5 1H GLY A 1120.758 11.050 -3.733 1.00 0.00 H ATOM 6 2H GLY A 1120.103 12.139 -2.617 1.00 0.00 H ATOM 7 3H GLY A 1119.180 10.832 -3.164 1.00 0.00 H ATOM 8 1HA GLY A 1121.737 10.331 -1.802 1.00 0.00 H ATOM 9 2HA GLY A 1120.312 10.720 -0.850 1.00 0.00 H ATOM10 N SER A 2121.135 7.935 -1.688 1.00 0.00 N ATOM11 CA SER A 2120.822 6.512 -1.752 1.00 0.00 C ATOM12 C SER A 2119.883 6.109 -0.621 1.00 0.00 C ATOM13 O SER A 2119.959 6.647 0.484 1.00 0.00 O ATOM14 CB SER A 2122.107 5.683 -1.684 1.00 0.00 C ATOM15 OG SER A 2122.628 5.441 -2.980 1.00 0.00 O ATOM16 H SER A 2122.055 8.214 -1.500 1.00 0.00 H ATOM17 HA SER A 2120.333 6.322 -2.695 1.00 0.00 H ATOM18 1HB SER A 2122.846 6.217 -1.107 1.00 0.00 H ATOM19 2HB SER A 2121.896 4.735 -1.211 1.00 0.00 H ATOM20 HG SER A 2122.628 6.259 -3.482 1.00 0.00 H ATOM21 N SER A 3118.997 5.160 -0.902 1.00 0.00 N ATOM22 CA SER A 3118.042 4.685 0.092 1.00 0.00 C ATOM23 C SER A 3118.645 3.564 0.933 1.00 0.00 C ATOM24 O SER A 3118.658 2.404 0.523 1.00 0.00 O ATOM25 CB SER A 3116.764 4.194 -0.591 1.00 0.00 C ATOM26 OG SER A 3117.063 3.463 -1.768 1.00 0.00 O ATOM27 H SER A 3118.986 4.769 -1.801 1.00 0.00 H ATOM28 HA SER A 3117.798 5.513 0.739 1.00 0.00 H ATOM29 1HB SER A 3116.220 3.553 0.087 1.00 0.00 H ATOM30 2HB SER A 3116.152 5.044 -0.854 1.00 0.00 H ATOM31 HG SER A 3117.138 4.068 -2.510 1.00 0.00 H

ATOM32 N GLY A 4119.143 3.920 2.114 1.00 0.00 N ATOM33 CA GLY A 4119.741 2.933 2.993 1.00 0.00 C ATOM34 C GLY A 4119.727 3.367 4.446 1.00 0.00 C ATOM35 O GLY A 4118.924 4.213 4.840 1.00 0.00 O ATOM36 H GLY A 4119.105 4.860 2.388 1.00 0.00 H ATOM37 1HA GLY A 4119.195 2.005 2.901 1.00 0.00 H ATOM38 2HA GLY A 4120.764 2.767 2.689 1.00 0.00 H ATOM39 N SER A 5120.616 2.785 5.244 1.00 0.00 N ATOM40 CA SER A 5120.703 3.116 6.662 1.00 0.00 C ATOM41 C SER A 5122.050 3.754 6.990 1.00 0.00 C ATOM42 O SER A 5122.125 4.697 7.777 1.00 0.00 O ATOM43 CB SER A 5120.499 1.861 7.513 1.00 0.00 C ATOM44 OG SER A 5119.829 2.169 8.723 1.00 0.00 O ATOM45 H SER A 5121.230 2.118 4.870 1.00 0.00 H ATOM46 HA SER A 5119.919 3.824 6.886 1.00 0.00 H ATOM47 1HB SER A 5119.907 1.147 6.961 1.00 0.00 H ATOM48 2HB SER A 5121.461 1.428 7.747 1.00 0.00 H ATOM49 HG SER A 5120.475 2.376 9.402 1.00 0.00 H ATOM50 N SER A 6123.109 3.233 6.381 1.00 0.00 N ATOM51 CA SER A 6124.454 3.751 6.607 1.00 0.00 C ATOM52 C SER A 6124.821 4.789 5.552 1.00 0.00 C ATOM53 O SER A 6124.732 4.528 4.353 1.00 0.00 O ATOM54 CB SER A 6125.472 2.611 6.594 1.00 0.00 C ATOM55 OG SER A 6126.514 2.846 7.526 1.00 0.00 O ATOM56 H SER A 6122.985 2.481 5.763 1.00 0.00 H ATOM57 HA SER A 6124.467 4.223 7.579 1.00 0.00 H ATOM58 1HB SER A 6124.978 1.686 6.853 1.00 0.00 H ATOM59 2HB SER A 6125.901 2.525 5.606 1.00 0.00 H ATOM60 HG SER A 6126.892 2.007 7.803 1.00 0.00 H ATOM61 N GLYA 7125.235 5.968 6.007 1.00 0.00 N ATOM62 CA GLY A 7125.610 7.027 5.088 1.00 0.00 C

ATOM63 C GLYA 7127.112 7.214 5.001 1.00 0.00 C ATOM64 O GLY A 7127.869 6.243 5.033 1.00 0.00 O ATOM65 H GLY A 7125.286 6.119 6.974 1.00 0.00 H ATOM66 1HA GLY A 7125.230 6.788 4.107 1.00 0.00 H ATOM67 2HA GLY A 7125.161 7.951 5.421 1.00 0.00 H ATOM68 N LEUA 8127.545 8.467 4.889 1.00 0.00 N ATOM69 CA LEU A 8128.966 8.780 4.795 1.00 0.00 C ATOM70 C LEUA 8129.559 8.221 3.505 1.00 0.00 C ATOM71 O LEUA 8130.682 7.717 3.493 1.00 0.00 O ATOM72 CB LEU A 8129.719 8.220 6.004 1.00 0.00 C ATOM73 CG LEU A 8129.030 8.435 7.352 1.00 0.00 C ATOM74 CD1 LEU A 8129.288 7.256 8.279 1.00 0.00 C ATOM75 CD2 LEU A 8129.506 9.731 7.991 1.00 0.00 C ATOM76 H LEUA 8126.893 9.197 4.867 1.00 0.00 H ATOM77 HA LEUA 8129.068 9.855 4.786 1.00 0.00 H ATOM78 1HB LEU A 8129.853 7.157 5.856 1.00 0.00 H ATOM79 2HB LEU A 8130.692 8.685 6.043 1.00 0.00 H ATOM80 HG LEU A 8127.964 8.510 7.196 1.00 0.00 H ATOM81 1HD1 LEU A 8129.004 7.522 9.286 1.00 0.00 H ATOM82 2HD1 LEU A 8130.337 7.002 8.254 1.00 0.00 H ATOM83 3HD1 LEU A 8128.704 6.408 7.952 1.00 0.00 H ATOM84 1HD2 LEU A 8130.301 9.516 8.691 1.00 0.00 H ATOM85 2HD2 LEU A 8128.684 10.199 8.512 1.00 0.00 H ATOM86 3HD2 LEU A 8129.872 10.397 7.224 1.00 0.00 H ATOM87 N ALAA 9128.795 8.314 2.423 1.00 0.00 N ATOM88 CA ALA A 9129.241 7.818 1.128 1.00 0.00 C ATOM89 C ALAA 9129.592 8.968 0.192 1.00 0.00 C ATOM90 O ALAA 9128.799 9.890 0.000 1.00 0.00 O ATOM91 CB ALA A 9128.171 6.934 0.504 1.00 0.00 C ATOM92 H ALAA 9127.908 8.725 2.497 1.00 0.00 H ATOM93 HA ALAA 9130.123 7.216 1.289 1.00 0.00 H

ATOM94 1HB ALA A 9127.782 6.258 1.251 1.00 0.00 H ATOM95 2HB ALA A 9128.602 6.365 -0.308 1.00 0.00 H ATOM96 3HB ALA A 9127.369 7.552 0.126 1.00 0.00 H ATOM97 N MET A 10130.785 8.908 -0.389 1.00 0.00 N ATOM98 CA MET A 10131.242 9.945 -1.306 1.00 0.00 C ATOM99 C MET A 10131.920 9.331 -2.528 1.00 0.00 C 100 O META 10133.135 9.442 -2.697 1.00 0.00 O **ATOM** 101 CB META 10132.206 10.896 -0.594 1.00 0.00 C **ATOM** 102 CG META 10131.568 11.663 0.553 1.00 0.00 C **ATOM** 103 SD MET A 10132.377 13.245 0.863 1.00 0.00 S 104 CE META 10132.247 14.013 -0.751 1.00 0.00 C **ATOM** 105 H META 10131.373 8.148 -0.197 1.00 0.00 H ATOM 106 HA META 10130.376 10.503 -1.632 1.00 0.00 H **ATOM** 107 1HB MET A 10133.031 10.321 -0.200 1.00 0.00 H **ATOM ATOM** 108 2HB MET A 10132.585 11.609 -1.310 1.00 0.00 H 109 1HG META 10130.531 11.846 0.314 1.00 0.00 H **ATOM** 110 2HG META 10131.629 11.062 1.448 1.00 0.00 H **ATOM** 111 1HE MET A 10133.228 14.073 -1.200 1.00 0.00 H ATOM 112 2HE MET A 10131.839 15.007 -0.644 1.00 0.00 H ATOM ATOM 113 3HE MET A 10131.598 13.422 -1.380 1.00 0.00 H 114 N PRO A 11131.139 8.673 -3.402 1.00 0.00 N ATOM 115 CA PRO A 11131.671 8.043 -4.613 1.00 0.00 C **ATOM** 116 C PRO A 11132.451 9.024 -5.486 1.00 0.00 C **ATOM** 117 O PRO A 11133.544 8.709 -5.957 1.00 0.00 O ATOM 118 CB PRO A 11130.423 7.547 -5.350 1.00 0.00 C **ATOM** 119 CG PRO A 11129.365 7.447 -4.304 1.00 0.00 C ATOM 120 CD PRO A 11129.682 8.497 -3.277 1.00 0.00 C **ATOM** 121 HA PRO A 11132.304 7.202 -4.372 1.00 0.00 H ATOM 122 1HB PRO A 11130.152 8.253 -6.120 1.00 0.00 H ATOM **ATOM** 123 2HB PRO A 11130.626 6.585 -5.795 1.00 0.00 H **ATOM** 124 1HG PRO A 11128.400 7.638 -4.744 1.00 0.00 H

125 2HG PRO A 11129.387 6.466 -3.855 1.00 0.00 H 126 1HD PRO A 11129.162 9.416 -3.504 1.00 0.00 H **ATOM** 127 2HD PRO A 11129.421 8.149 -2.288 1.00 0.00 H **ATOM** 128 N PRO A 12131.907 10.235 -5.713 1.00 0.00 N ATOM ATOM 129 CA PRO A 12132.573 11.253 -6.531 1.00 0.00 C 130 C PRO A 12133.937 11.637 -5.966 1.00 0.00 C ATOM ATOM 131 O PRO A 12134.781 12.188 -6.673 1.00 0.00 O ATOM 132 CB PRO A 12131.618 12.453 -6.477 1.00 0.00 C 133 CG PRO A 12130.301 11.882 -6.078 1.00 0.00 C ATOM 134 CD PRO A 12130.613 10.712 -5.191 1.00 0.00 C **ATOM** 135 HA PRO A 12132.688 10.926 -7.553 1.00 0.00 H ATOM **ATOM** 136 1HB PRO A 12131.975 13.167 -5.750 1.00 0.00 H 137 2HB PRO A 12131.566 12.918 -7.451 1.00 0.00 H ATOM **ATOM** 138 1HG PRO A 12129.729 12.621 -5.537 1.00 0.00 H ATOM 139 2HG PRO A 12129.761 11.555 -6.954 1.00 0.00 H **ATOM** 140 1HD PRO A 12130.705 11.030 -4.163 1.00 0.00 H 141 2HD PRO A 12129.854 9.952 -5.287 1.00 0.00 H ATOM 142 N GLY A 13134.145 11.341 -4.687 1.00 0.00 N ATOM ATOM 143 CA GLY A 13135.408 11.661 -4.048 1.00 0.00 C 144 C GLY A 13136.522 10.720 -4.461 1.00 0.00 C ATOM ATOM 145 O GLYA 13137.189 10.944 -5.472 1.00 0.00 O 146 H GLY A 13133.435 10.900 -4.171 1.00 0.00 H ATOM ATOM 147 1HA GLY A 13135.687 12.670 -4.313 1.00 0.00 H 148 2HA GLY A 13135.282 11.603 -2.977 1.00 0.00 H ATOM 149 N ASNA 14136.723 9.665 -3.678 1.00 0.00 N **ATOM** 150 CA ASN A 14137.765 8.687 -3.969 1.00 0.00 C ATOM 151 C ASNA 14137.162 7.396 -4.514 1.00 0.00 C ATOM 152 O ASN A 14137.556 6.914 -5.575 1.00 0.00 O ATOM 153 CB ASN A 14138.580 8.389 -2.709 1.00 0.00 C ATOM 154 CG ASN A 14139.257 9.626 -2.152 1.00 0.00 C ATOM 155 OD1 ASN A 14140.304 10.048 -2.643 1.00 0.00 O ATOM

- ATOM 156 ND2 ASN A 14138.660 10.215 -1.122 1.00 0.00 N
- ATOM 157 H ASN A 14136.159 9.542 -2.887 1.00 0.00 H
- ATOM 158 HA ASN A 14138.418 9.109 -4.718 1.00 0.00 H
- ATOM 159 1HB ASN A 14137.925 7.988 -1.950 1.00 0.00 H
- ATOM 160 2HB ASN A 14139.341 7.660 -2.944 1.00 0.00 H
- ATOM 161 1HD2 ASN A 14137.829 9.823 -0.784 1.00 0.00 H
- ATOM 162 2HD2 ASN A 14139.076 11.018 -0.744 1.00 0.00 H
- ATOM 163 N SER A 15136.202 6.842 -3.779 1.00 0.00 N
- ATOM 164 CA SER A 15135.544 5.607 -4.189 1.00 0.00 C
- ATOM 165 C SER A 15134.436 5.233 -3.208 1.00 0.00 C
- ATOM 166 O SER A 15133.344 4.832 -3.612 1.00 0.00 O
- ATOM 167 CB SER A 15136.561 4.468 -4.286 1.00 0.00 C
- ATOM 168 OG SER A 15137.099 4.375 -5.592 1.00 0.00 O
- ATOM 169 H SER A 15135.930 7.274 -2.943 1.00 0.00 H
- ATOM 170 HA SER A 15135.106 5.770 -5.163 1.00 0.00 H
- ATOM 171 1HB SER A 15137.366 4.649 -3.590 1.00 0.00 H
- ATOM 172 2HB SER A 15136.076 3.535 -4.041 1.00 0.00 H
- ATOM 173 HG SER A 15136.766 3.582 -6.020 1.00 0.00 H
- ATOM 174 N HIS A 16134.726 5.365 -1.919 1.00 0.00 N
- ATOM 175 CA HIS A 16133.756 5.041 -0.879 1.00 0.00 C
- ATOM 176 C HIS A 16134.196 5.603 0.468 1.00 0.00 C
- ATOM 177 O HIS A 16133.479 6.389 1.089 1.00 0.00 O
- ATOM 178 CB HIS A 16133.574 3.525 -0.778 1.00 0.00 C
- ATOM 179 CG HIS A 16132.466 2.998 -1.636 1.00 0.00 C
- ATOM 180 ND1 HIS A 16131.131 3.188 -1.343 1.00 0.00 N
- ATOM 181 CD2 HIS A 16132.499 2.283 -2.786 1.00 0.00 C
- ATOM 182 CE1 HIS A 16130.392 2.611 -2.275 1.00 0.00 C
- ATOM 183 NE2 HIS A 16131.198 2.057 -3.162 1.00 0.00 N
- ATOM 184 H HIS A 16135.614 5.688 -1.660 1.00 0.00 H
- ATOM 185 HA HIS A 16132.814 5.491 -1.153 1.00 0.00 H
- ATOM 186 1HB HIS A 16134.489 3.038 -1.081 1.00 0.00 H

187 2HB HIS A 16133.355 3.264 0.247 1.00 0.00 H **ATOM** 188 HD1 HIS A 16130.779 3.672 -0.567 1.00 0.00 H **ATOM ATOM** 189 HD2 HIS A 16133.384 1.952 -3.310 1.00 0.00 H **ATOM** 190 HE1 HIS A 16129.313 2.598 -2.306 1.00 0.00 H 191 HE2 HIS A 16130.911 1.498 -3.913 1.00 0.00 H **ATOM** 192 N GLY A 17135.381 5.198 0.914 1.00 0.00 N **ATOM** 193 CA GLY A 17135.896 5.673 2.185 1.00 0.00 C ATOM 194 C GLY A 17137.255 5.085 2.515 1.00 0.00 C **ATOM** 195 O GLY A 17137.399 4.345 3.488 1.00 0.00 O **ATOM** 196 H GLY A 17135.909 4.572 0.377 1.00 0.00 H **ATOM** 197 1HA GLY A 17135.981 6.748 2.148 1.00 0.00 H **ATOM** 198 2HA GLY A 17135,201 5,403 2,967 1.00 0.00 H ATOM **ATOM** 199 N LEUA 18138.253 5.417 1.703 1.00 0.00 N 200 CA LEU A 18139.607 4.918 1.913 1.00 0.00 C ATOM 201 C LEU A 18140.527 6.030 2.407 1.00 0.00 C **ATOM** 202 O LEUA 18140.851 6.956 1.663 1.00 0.00 O ATOM 203 CB LEU A 18140.160 4.320 0.618 1.00 0.00 C **ATOM** 204 CG LEU A 18139.326 3.186 0.021 1.00 0.00 C ATOM 205 CD1 LEU A 18139.476 3.153 -1.493 1.00 0.00 C **ATOM** 206 CD2 LEU A 18139.730 1.851 0.628 1.00 0.00 C **ATOM** ATOM 207 H LEU A 18138.075 6.012 0.944 1.00 0.00 H 208 HA LEUA 18139.562 4.144 2.665 1.00 0.00 H ATOM 209 1HB LEU A 18140.234 5.111 -0.115 1.00 0.00 H **ATOM ATOM** 210 2HB LEU A 18141.151 3.942 0.815 1.00 0.00 H 211 HG LEU A 18138.283 3.356 0.248 1.00 0.00 H ATOM **ATOM** 212 1HD1 LEU A 18139.372 2.136 -1.842 1.00 0.00 H 213 2HD1 LEU A 18140.451 3.528 -1.766 1.00 0.00 H ATOM 214 3HD1 LEU A 18138.713 3.768 -1.944 1.00 0.00 H ATOM 215 1HD2 LEU A 18140.757 1.903 0.959 1.00 0.00 H ATOM 216 2HD2 LEU A 18139.629 1.073 -0.113 1.00 0.00 H ATOM 217 3HD2 LEU A 18139.092 1.630 1.471 1.00 0.00 H ATOM

ATOM 218 N GLU A 19140.945 5.931 3.664 1.00 0.00 N ATOM ,219 CA GLU A 19141.830 6.927 4.257 1.00 0.00 C ATOM 220 C GLU A 19142.859 6.267 5.168 1.00 0.00 C 221 O GLUA 19142.811 5.059 5.403 1.00 0.00 O ATOM ATOM 222 CB GLU A 19141.017 7.954 5.047 1.00 0.00 C ATOM 223 CG GLU A 19140.018 7.331 6.010 1.00 0.00 C 224 CD GLU A 19138.580 7.626 5.632 1.00 0.00 C ATOM **ATOM** 225 OE1 GLU A 19138.293 8.777 5.240 1.00 0.00 O **ATOM** 226 OE2 GLU A 19137.741 6.705 5.727 1.00 0.00 O 227 H GLU A 19140.653 5.168 4.207 1.00 0.00 H **ATOM** 228 HA GLU A 19142.347 7.431 3.454 1.00 0.00 H **ATOM** 229 1HB GLU A 19141.696 8.573 5.617 1.00 0.00 H ATOM 230 2HB GLU A 19140.474 8.579 4.353 1.00 0.00 H ATOM ATOM 231 1HG GLUA 19140.161 6.261 6.013 1.00 0.00 H 232 2HG GLU A 19140.202 7.721 7.000 1.00 0.00 H ATOM 233 N VALA 20143.791 7.066 5.679 1.00 0.00 N ATOM **ATOM** 234 CA VALA 20144.831 6.559 6.564 1.00 0.00 C 235 C VALA 20144.232 5.988 7.845 1.00 0.00 C ATOM 236 O VALA 20143.373 6.610 8.471 1.00 0.00 O **ATOM** 237 CB VALA 20145.845 7.660 6.930 1.00 0.00 C ATOM 238 CG1 VAL A 20147.003 7.079 7.729 1.00 0.00 C **ATOM** 239 CG2 VAL A 20146.352 8.359 5.677 1.00 0.00 C **ATOM** 240 H VALA 20143.776 8.020 5.455 1.00 0.00 H **ATOM** ATOM 241 HA VALA 20145.358 5.773 6.043 1.00 0.00 H **ATOM** 242 HB VALA 20145.345 8.392 7.547 1.00 0.00 H 243 1HG1 VAL A 20147.813 7.792 7.760 1.00 0.00 H **ATOM** 244 2HG1 VAL A 20147.342 6.167 7.260 1.00 0.00 H **ATOM** 245 3HG1 VAL A 20146.674 6.864 8.735 1.00 0.00 H **ATOM** 246 1HG2 VAL A 20146.407 9.423 5.856 1.00 0.00 H ATOM **ATOM** 247 2HG2 VAL A 20145.676 8.167 4.858 1.00 0.00 H ATOM 248 3HG2 VAL A 20147.335 7.985 5.429 1.00 0.00 H

249 N GLYA 21144.691 4.802 8.230 1.00 0.00 N 250 CA GLY A 21144.189 4.168 9.435 1.00 0.00 C ATOM 251 C GLY A 21143.139 3.114 9.141 1.00 0.00 C ATOM 252 O GLY A 21142.996 2.145 9.887 1.00 0.00 O ATOM 253 H GLY A 21145.376 4.354 7.691 1.00 0.00 H **ATOM** 254 1HA GLY A 21145.013 3.703 9.954 1.00 0.00 H ATOM 255 2HA GLY A 21143.756 4.923 10.072 1.00 0.00 H ATOM 256 N SER A 22142.400 3.304 8.051 1.00 0.00 N ATOM **ATOM** 257 CA SER A 22141.358 2.363 7.661 1.00 0.00 C 258 C SER A 22141.934 1.233 6.815 1.00 0.00 C **ATOM** 259 O SER A 22142.916 1.420 6.095 1.00 0.00 O ATOM 260 CB SER A 22140.255 3.084 6.886 1.00 0.00 C **ATOM** 261 OG SER A 22139.291 3.639 7.764 1.00 0.00 O ATOM 262 H SER A 22142.561 4.097 7.498 1.00 0.00 H ATOM 263 HA SER A 22140.936 1.943 8.563 1.00 0.00 H ATOM 264 1HB SER A 22140.690 3.882 6.302 1.00 0.00 H ATOM ATOM 265 2HB SER A 22139.763 2.384 6.227 1.00 0.00 H 266 HG SER A 22139.736 4.075 8.494 1.00 0.00 H ATOM 267 N LEUA 23141.319 0.059 6.906 1.00 0.00 N ATOM 268 CA LEU A 23141.771 -1.103 6.149 1.00 0.00 C ATOM ATOM 269 C LEUA 23141.219 -1.074 4.727 1.00 0.00 C 270 O LEUA 23140.087 -0.646 4.499 1.00 0.00 O ATOM 271 CB LEU A 23141.341 -2.394 6.849 1.00 0.00 C ATOM 272 CG LEU A 23142.012 -2.651 8.199 1.00 0.00 C ATOM 273 CD1 LEU A 23141.094 -3.458 9.106 1.00 0.00 C ATOM 274 CD2 LEU A 23143.339 -3.369 8.005 1.00 0.00 C ATOM **ATOM** 275 H LEUA 23140.542 -0.029 7.497 1.00 0.00 H 276 HA LEU A 23142.849 -1.070 6.104 1.00 0.00 H ATOM 277 1HB LEU A 23140.273 -2.356 7.002 1.00 0.00 H **ATOM** 278 2HB LEU A 23141.566 -3.224 6.197 1.00 0.00 H ATOM ATOM 279 HG LEU A 23142.211 -1.706 8.682 1.00 0.00 H

280 1HD1 LEU A 23140.445 -4.074 8.503 1.00 0.00 H ATOM 281 2HD1 LEU A 23140.499 -2.784 9.705 1.00 0.00 H **ATOM** 282 3HD1 LEU A 23141.689 -4.085 9.753 1.00 0.00 H **ATOM** 283 1HD2 LEU A 23143.169 -4.436 7.969 1.00 0.00 H **ATOM** 284 2HD2 LEU A 23143.997 -3.138 8.830 1.00 0.00 H **ATOM** 285 3HD2 LEU A 23143.792 -3.046 7.080 1.00 0.00 H ATOM 286 N ALAA 24142.025 -1.531 3.776 1.00 0.00 N **ATOM** 287 CA ALAA 24141.617 -1.558 2.376 1.00 0.00 C **ATOM** 288 C ALAA 24142.162 -2.794 1.669 1.00 0.00 C ATOM 289 O ALAA 24143.002 -3.511 2.211 1.00 0.00 O ATOM 290 CB ALAA 24142.082 -0.294 1.668 1.00 0.00 C ATOM 291 H ALAA 24142.916 -1.859 4.019 1.00 0.00 H **ATOM** 292 HA ALAA 24140.538 -1.584 2.345 1.00 0.00 H ATOM 293 1HB ALA A 24143.093 -0.432 1.314 1.00 0.00 H ATOM 294 2HB ALA A 24142.051 0.537 2.357 1.00 0.00 H ATOM 295 3HB ALAA 24141.432 -0.091 0.830 1.00 0.00 H **ATOM** 296 N GLUA 25141.678 -3.036 0.456 1.00 0.00 N **ATOM** 297 CA GLUA 25142.117 -4.186 -0.326 1.00 0.00 C ATOM 298 C GLUA 25142.455 -3.774 -1.756 1.00 0.00 C **ATOM** 299 O GLUA 25141.823 -2.884 -2.323 1.00 0.00 O ATOM 300 CB GLU A 25141.032 -5.265 -0.338 1.00 0.00 C **ATOM** 301 CG GLU A 25141.479 -6.569 -0.978 1.00 0.00 C ATOM 302 CD GLU A 25140.325 -7.520 -1.231 1.00 0.00 C **ATOM** 303 OE1 GLU A 25140.422 -8.335 -2.172 1.00 0.00 O ATOM 304 OE2 GLU A 25139.324 -7.450 -0.486 1.00 0.00 O **ATOM** 305 H GLUA 25141.010 -2.427 0.076 1.00 0.00 H **ATOM** 306 HA GLU A 25143.004 -4.585 0.140 1.00 0.00 H **ATOM** 307 1HB GLU A 25140.736 -5.472 0.680 1.00 0.00 H **ATOM** 308 2HB GLU A 25140.178 -4.896 -0.885 1.00 0.00 H **ATOM** 309 1HG GLU A 25141.955 -6.348 -1.921 1.00 0.00 H **ATOM** 310 2HG GLU A 25142.188 -7.053 -0.323 1.00 0.00 H

- ATOM 311 N VALA 26143.459 -4.429 -2.333 1.00 0.00 N
- ATOM 312 CA VAL A 26143.882 -4.131 -3.695 1.00 0.00 C
- ATOM 313 C VALA 26143.519 -5.267 -4.644 1.00 0.00 C
- ATOM 314 O VALA 26143.657 -6.442 -4.305 1.00 0.00 O
- ATOM 315 CB VALA 26145.400 -3.881 -3.770 1.00 0.00 C
- ATOM 316 CG1 VAL A 26145.791 -3.373 -5.149 1.00 0.00 C
- ATOM 317 CG2 VAL A 26145.833 -2.901 -2.690 1.00 0.00 C
- ATOM 318 H VALA 26143.925 -5.129 -1.829 1.00 0.00 H
- ATOM 319 HA VALA 26143.374 -3.233 -4.014 1.00 0.00 H
- ATOM 320 HB VALA 26145.908 -4.819 -3.600 1.00 0.00 H
- ATOM 321 1HG1 VAL A 26145.889 -2.297 -5.123 1.00 0.00 H
- ATOM 322 2HG1 VAL A 26145.030 -3.648 -5.864 1.00 0.00 H
- ATOM 323 3HG1 VAL A 26146.734 -3.812 -5.440 1.00 0.00 H
- ATOM 324 1HG2 VAL A 26145.367 -3.169 -1.753 1.00 0.00 H
- ATOM 325 2HG2 VAL A 26145.533 -1.902 -2.968 1.00 0.00 H
- ATOM 326 3HG2 VAL A 26146.907 -2.938 -2.582 1.00 0.00 H
- ATOM 327 N LYS A 27143.052 -4.909 -5.837 1.00 0.00 N
- ATOM 328 CA LYS A 27142.669 -5.900 -6.836 1.00 0.00 C
- ATOM 329 C LYS A 27143.868 -6.308 -7.685 1.00 0.00 C
- ATOM 330 O LYS A 27144.189 -5.657 -8.680 1.00 0.00 O
- ATOM 331 CB LYS A 27141.557 -5.347 -7.731 1.00 0.00 C
- ATOM 332 CG LYS A 27140.454 -6.352 -8.020 1.00 0.00 C
- ATOM 333 CD LYS A 27139.652 -6.674 -6.770 1.00 0.00 C
- ATOM 334 CE LYS A 27138.931 -5.445 -6.239 1.00 0.00 C
- ATOM 335 NZ LYS A 27139.738 -4.727 -5.213 1.00 0.00 N
- ATOM 336 H LYS A 27142.964 -3.957 -6.049 1.00 0.00 H
- ATOM 337 HA LYS A 27142.299 -6.770 -6.315 1.00 0.00 H
- ATOM 338 1HB LYS A 27141.115 -4.489 -7.248 1.00 0.00 H
- ATOM 339 2HB LYS A 27141.988 -5.037 -8.672 1.00 0.00 H
- ATOM 340 1HG LYS A 27139.790 -5.939 -8.765 1.00 0.00 H
- ATOM 341 2HG LYS A 27140.898 -7.262 -8.397 1.00 0.00 H

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342 1HD LYS A 27138.922 -7.433 -7.007 1.00 0.00 H
       343 2HD LYS A 27140.324 -7.043 -6.008 1.00 0.00 H
ATOM
       344 1HE LYS A 27138.735 -4.775 -7.063 1.00 0.00 H
ATOM
       345 2HE LYS A 27137.996 -5.755 -5.797 1.00 0.00 H
ATOM
       346 1HZ LYS A 27140.748 -4.947 -5.335 1.00 0.00 H
ATOM
       347 2HZ LYS A 27139.443 -5.018 -4.260 1.00 0.00 H
ATOM
ATOM
       348 3HZ LYS A 27139.603 -3.701 -5.308 1.00 0.00 H
       349 N GLUA 28144.529 -7.390 -7.286 1.00 0.00 N
ATOM
       350 CA GLUA 28145.694 -7.886 -8.010 1.00 0.00 C
ATOM
       351 C GLUA 28145.709 -9.411 -8.036 1.00 0.00 C
ATOM
       352 O GLUA 28144.797 -10.059 -7.525 1.00 0.00 O
ATOM
       353 CB GLUA 28146.980 -7.360 -7.368 1.00 0.00 C
ATOM
       354 CG GLUA 28147.981 -6.812 -8.372 1.00 0.00 C
ATOM
       355 CD GLUA 28149.350 -6.580 -7.762 1.00 0.00 C
ATOM
       356 OE1 GLU A 28149.538 -5.534 -7.106 1.00 0.00 O
ATOM
       357 OE2 GLU A 28150.233 -7.446 -7.941 1.00 0.00 O
ATOM
ATOM
       358 H GLUA 28144.225 -7.867 -6.485 1.00 0.00 H
       359 HA GLUA 28145.633 -7.520 -9.024 1.00 0.00 H
ATOM
       360 1HB GLU A 28146.727 -6.570 -6.677 1.00 0.00 H
ATOM
       361 2HB GLU A 28147.453 -8.164 -6.824 1.00 0.00 H
ATOM
       362 1HG GLU A 28148.080 -7.517 -9.183 1.00 0.00 H
ATOM
ATOM
        363 2HG GLU A 28147.609 -5.873 -8.755 1.00 0.00 H
       364 N ASNA 29146.752 -9.977 -8.635 1.00 0.00 N
ATOM
        365 CA ASN A 29146.886 -11.426 -8.726 1.00 0.00 C
ATOM
        366 C ASN A 29146.958 -12.052 -7.335 1.00 0.00 C
ATOM
       367 O ASN A 29146.123 -12.880 -6.974 1.00 0.00 O
ATOM
       368 CB ASN A 29148.133 -11.794 -9.533 1.00 0.00 C
ATOM
        369 CG ASN A 29147.812 -12.105 -10.982 1.00 0.00 C
ATOM
        370 OD1 ASN A 29147.758 -13.268 -11.382 1.00 0.00 O
ATOM
       371 ND2 ASN A 29147.598 -11.063 -11.777 1.00 0.00 N
ATOM
       372 H ASN A 29147.448 -9.407 -9.023 1.00 0.00 H
ATOM
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- ATOM 373 HA ASN A 29146.013 -11.808 -9.235 1.00 0.00 H
- ATOM 374 1HB ASN A 29148.828 -10.969 -9.507 1.00 0.00 H
- ATOM 375 2HB ASN A 29148.597 -12.664 -9.092 1.00 0.00 H
- ATOM 376 1HD2 ASN A 29147.658 -10.166 -11.389 1.00 0.00 H
- ATOM 377 2HD2 ASN A 29147.388 -11.235 -12.719 1.00 0.00 H
- ATOM 378 N PRO A 30147.964 -11.661 -6.533 1.00 0.00 N
- ATOM 379 CA PRO A 30148.142 -12.186 -5.177 1.00 0.00 C
- ATOM 380 C PRO A 30147.167 -11.559 -4.180 1.00 0.00 C
- ATOM 381 O PRO A 30147.291 -10.383 -3.839 1.00 0.00 O
- ATOM 382 CB PRO A 30149.577 -11.785 -4.840 1.00 0.00 C
- ATOM 383 CG PRO A 30149.809 -10.537 -5.617 1.00 0.00 C
- ATOM 384 CD PRO A 30149.006 -10.676 -6.885 1.00 0.00 C
- ATOM 385 HA PRO A 30148.048 -13.261 -5.151 1.00 0.00 H
- ATOM 386 1HB PRO A 30149.666 -11.614 -3.777 1.00 0.00 H
- ATOM 387 2HB PRO A 30150.254 -12.571 -5.143 1.00 0.00 H
- ATOM 388 1HG PRO A 30149.468 -9.684 -5.050 1.00 0.00 H
- ATOM 389 2HG PRO A 30150.859 -10.438 -5.849 1.00 0.00 H
- ATOM 390 1HD PRO A 30148.564 -9.730 -7.156 1.00 0.00 H
- ATOM 391 2HD PRO A 30149.628 -11.045 -7.685 1.00 0.00 H
- ATOM 392 N PRO A 31146.181 -12.338 -3.697 1.00 0.00 N
- ATOM 393 CA PRO A 31145.190 -11.843 -2.736 1.00 0.00 C
- ATOM 394 C PRO A 31145.794 -11.586 -1.360 1.00 0.00 C
- ATOM 395 O PRO A 31146.067 -12.521 -0.606 1.00 0.00 O
- ATOM 396 CB PRO A 31144.165 -12.976 -2.667 1.00 0.00 C
- ATOM 397 CG PRO A 31144.925 -14.198 -3.043 1.00 0.00 C
- ATOM 398 CD PRO A 31145.955 -13.754 -4.044 1.00 0.00 C
- ATOM 399 HA PRO A 31144.712 -10.941 -3.091 1.00 0.00 H
- ATOM 400 1HB PRO A 31143.770 -13.047 -1.663 1.00 0.00 H
- ATOM 401 2HB PRO A 31143.361 -12.782 -3.362 1.00 0.00 H
- ATOM 402 1HG PRO A 31145.408 -14.615 -2.170 1.00 0.00 H
- ATOM 403 2HG PRO A 31144.260 -14.924 -3.487 1.00 0.00 H

404 1HD PRO A 31146.863 -14.327 -3.934 1.00 0.00 H **ATOM** 405 2HD PRO A 31145.569 -13.846 -5.048 1.00 0.00 H **ATOM** 406 N PHE A 32146.001 -10.313 -1.038 1.00 0.00 N 407 CA PHE A 32146.574 -9.933 0.248 1.00 0.00 C ATOM 408 C PHE A 32145.715 -8.877 0.935 1.00 0.00 C ATOM ATOM 409 O PHE A 32144.802 -8.315 0.330 1.00 0.00 O 410 CB PHE A 32147.998 -9.406 0.061 1.00 0.00 C ATOM 411 CG PHE A 32148.118 -8.373 -1.023 1.00 0.00 C **ATOM** 412 CD1 PHE A 32148.820 -8.648 -2.186 1.00 0.00 C ATOM 413 CD2 PHE A 32147.530 -7.127 -0.877 1.00 0.00 C ATOM 414 CE1 PHE A 32148.933 -7.700 -3.184 1.00 0.00 C ATOM 415 CE2 PHE A 32147.641 -6.173 -1.873 1.00 0.00 C ATOM 416 CZ PHE A 32148.342 -6.460 -3.028 1.00 0.00 C ATOM 417 H PHE A 32145.764 -9.613 -1.680 1.00 0.00 H ATOM 418 HA PHE A 32146.606 -10.815 0.870 1.00 0.00 H ATOM 419 1HB PHE A 32148.333 -8.959 0.985 1.00 0.00 H ATOM 420 2HB PHE A 32148.649 -10.231 -0.190 1.00 0.00 H ATOM 421 HD1 PHE A 32149.281 -9.617 -2.308 1.00 0.00 H ATOM 422 HD2 PHE A 32146.982 -6.901 0.025 1.00 0.00 H **ATOM** 423 HE1 PHE A 32149.483 -7.927 -4.086 1.00 0.00 H ATOM 424 HE2 PHE A 32147.178 -5.206 -1.748 1.00 0.00 H **ATOM** 425 HZ PHE A 32148.429 -5.718 -3.807 1.00 0.00 H ATOM 426 N TYR A 33146.012 -8.612 2.203 1.00 0.00 N ATOM 427 CA TYR A 33145.266 -7.623 2.973 1.00 0.00 C ATOM 428 C TYR A 33146.213 -6.681 3.708 1.00 0.00 C ATOM 429 O TYR A 33147.222 -7.110 4.269 1.00 0.00 O ATOM 430 CB TYR A 33144.340 -8.318 3.973 1.00 0.00 C ATOM 431 CG TYR A 33143.079 -8.869 3.348 1.00 0.00 C **ATOM** 432 CD1 TYR A 33142.709 -10.196 3.538 1.00 0.00 C ATOM ATOM 433 CD2 TYR A 33142.257 -8.064 2.568 1.00 0.00 C ATOM 434 CE1 TYR A 33141.557 -10.703 2.969 1.00 0.00 C

- ATOM 435 CE2 TYR A 33141.103 -8.566 1.996 1.00 0.00 C
- ATOM 436 CZ TYR A 33140.758 -9.885 2.199 1.00 0.00 C
- ATOM 437 OH TYR A 33139.610 -10.387 1.630 1.00 0.00 O
- ATOM 438 H TYR A 33146.751 -9.094 2.631 1.00 0.00 H
- ATOM 439 HA TYR A 33144.669 -7.047 2.282 1.00 0.00 H
- ATOM 440 1HB TYR A 33144.869 -9.139 4.432 1.00 0.00 H
- ATOM 441 2HB TYR A 33144.051 -7.610 4.736 1.00 0.00 H
- ATOM 442 HD1 TYR A 33143.337 -10.833 4.141 1.00 0.00 H
- ATOM 443 HD2 TYR A 33142.531 -7.032 2.411 1.00 0.00 H
- ATOM 444 HE1 TYR A 33141.286 -11.737 3.127 1.00 0.00 H
- ATOM 445 HE2 TYR A 33140.477 -7.924 1.393 1.00 0.00 H
- ATOM 446 HH TYR A 33139.802 -11.228 1.209 1.00 0.00 H
- ATOM 447 N GLY A 34145.881 -5.394 3.704 1.00 0.00 N
- ATOM 448 CA GLY A 34146.711 -4.411 4.374 1.00 0.00 C
- ATOM 449 C GLY A 34145.948 -3.149 4.725 1.00 0.00 C
- ATOM 450 O GLY A 34144.896 -2.873 4.150 1.00 0.00 O
- ATOM 451 H GLY A 34145.066 -5.109 3.241 1.00 0.00 H
- ATOM 452 1HA GLY A 34147.103 -4.846 5.282 1.00 0.00 H
- ATOM 453 2HA GLY A 34147.537 -4.151 3.727 1.00 0.00 H
- ATOM 454 N VALA 35146.480 -2.382 5.671 1.00 0.00 N
- ATOM 455 CA VAL A 35145.842 -1.143 6.098 1.00 0.00 C
- ATOM 456 C VALA 35146.536 0.070 5.486 1.00 0.00 C
- ATOM 457 O VALA 35147.743 0.052 5.247 1.00 0.00 O
- ATOM 458 CB VALA 35145.848 -1.009 7.635 1.00 0.00 C
- ATOM 459 CG1 VAL A 35147.273 -0.996 8.169 1.00 0.00 C
- ATOM 460 CG2 VAL A 35145.095 0.240 8.067 1.00 0.00 C
- ATOM 461 H VALA 35147.322 -2.656 6.092 1.00 0.00 H
- ATOM 462 HA VALA 35144.816 -1.165 5.763 1.00 0.00 H
- ATOM 463 HB VALA 35145.342 -1.869 8.050 1.00 0.00 H
- ATOM 464 1HG1 VAL A 35147.344 -0.295 8.987 1.00 0.00 H
- ATOM 465 2HG1 VAL A 35147.950 -0.699 7.381 1.00 0.00 H

466 3HG1 VAL A 35147.536 -1.984 8.516 1.00 0.00 H ATOM **ATOM** 467 1HG2 VAL A 35145.576 1.113 7.652 1.00 0.00 H 468 2HG2 VAL A 35145.096 0.307 9.145 1.00 0.00 H **ATOM ATOM** 469 3HG2 VALA 35144.076 0.188 7.712 1.00 0.00 H 470 N ILE A 36145.764 1.122 5.233 1.00 0.00 N **ATOM** 471 CA ILE A 36146.305 2.343 4.648 1.00 0.00 C **ATOM** 472 C ILE A 36147.257 3.039 5.615 1.00 0.00 C **ATOM** ATOM 473 O ILEA 36147.061 3.001 6.830 1.00 0.00 O 474 CB ILE A 36145.182 3.324 4.253 1.00 0.00 C **ATOM** 475 CG1 ILE A 36144.129 2.611 3.400 1.00 0.00 C ATOM 476 CG2 ILE A 36145.758 4.516 3.505 1.00 0.00 C **ATOM** 477 CD1 ILE A 36142.990 3.510 2.971 1.00 0.00 C ATOM ATOM 478 H ILE A 36144.808 1.075 5.445 1.00 0.00 H 479 HA ILE A 36146.848 2.073 3.754 1.00 0.00 H ATOM 480 HB ILE A 36144.717 3.687 5.157 1.00 0.00 H **ATOM** 481 1HG1 ILE A 36144.599 2.224 2.509 1.00 0.00 H ATOM 482 2HG1 ILE A 36143.711 1.791 3.967 1.00 0.00 H ATOM ATOM 483 1HG2 ILE A 36146.253 5.174 4.204 1.00 0.00 H 484 2HG2 ILE A 36144.960 5.051 3.011 1.00 0.00 H ATOM 485 3HG2 ILE A 36146.469 4.172 2.770 1.00 0.00 H ATOM 486 1HD1 ILE A 36142.253 3.558 3.759 1.00 0.00 H ATOM 487 2HD1 ILE A 36142.535 3.111 2.076 1.00 0.00 H ATOM 488 3HD1 ILE A 36143.369 4.500 2.772 1.00 0.00 H ATOM 489 N ARG A 37148.287 3.674 5.067 1.00 0.00 N ATOM 490 CA ARG A 37149.271 4.379 5.882 1.00 0.00 C ATOM 491 C ARG A 37149.476 5.804 5.378 1.00 0.00 C **ATOM** 492 O ARGA 37149.174 6.769 6.080 1.00 0.00 O ATOM 493 CB ARG A 37150.604 3.626 5.872 1.00 0.00 C ATOM 494 CG ARG A 37150.463 2.137 6.139 1.00 0.00 C ATOM 495 CD ARG A 37149.863 1.870 7.511 1.00 0.00 C ATOM ATOM 496 NE ARG A 37150.865 1.945 8.571 1.00 0.00 N

ATOM 497 CZ ARG A 37150.616 1.661 9.847 1.00 0.00 C 498 NH1 ARG A 37149.401 1.284 10.226 1.00 0.00 N ATOM 499 NH2 ARG A 37151.585 1.755 10.749 1.00 0.00 N ATOM 500 H ARG A 37148.389 3.668 4.093 1.00 0.00 H **ATOM** 501 HA ARG A 37148.897 4.418 6.893 1.00 0.00 H ATOM 502 1HB ARG A 37151.069 3.754 4.907 1.00 0.00 H ATOM 503 2HB ARG A 37151.247 4.047 6.632 1.00 0.00 H ATOM 504 1HG ARG A 37149.820 1.705 5.386 1.00 0.00 H ATOM **ATOM** 505 2HG ARG A 37151.440 1.678 6.088 1.00 0.00 H 506 1HD ARG A 37149.095 2.605 7.702 1.00 0.00 H **ATOM ATOM** 507 2HD ARG A 37149.424 0.883 7.511 1.00 0.00 H 508 HE ARG A 37151.770 2.221 8.319 1.00 0.00 H **ATOM** 509 1HH1 ARG A 37148.667 1.211 9.551 1.00 0.00 H ATOM 510 2HH1 ARG A 37149.221 1.071 11.187 1.00 0.00 H ATOM 511 1HH2 ARG A 37152.502 2.039 10.469 1.00 0.00 H **ATOM** 512 2HH2 ARG A 37151.398 1.542 11.707 1.00 0.00 H ATOM **ATOM** 513 N TRP A 38149.989 5.929 4.158 1.00 0.00 N ATOM 514 CA TRPA 38150.233 7.238 3.563 1.00 0.00 C 515 C TRP A 38149.491 7.382 2.237 1.00 0.00 C **ATOM** 516 O TRPA 38149.514 6.481 1.399 1.00 0.00 O ATOM 517 CB TRPA 38151.735 7.456 3.349 1.00 0.00 C ATOM 518 CG TRPA 38152.054 8.673 2.533 1.00 0.00 C ATOM 519 CD1 TRP A 38152.277 9.938 2.997 1.00 0.00 C **ATOM** 520 CD2 TRP A 38152.180 8.741 1.107 1.00 0.00 C ATOM 521 NE1 TRP A 38152.534 10.787 1.947 1.00 0.00 N **ATOM** 522 CE2 TRP A 38152.480 10.075 0.777 1.00 0.00 C ATOM 523 CE3 TRP A 38152.068 7.801 0.079 1.00 0.00 C ATOM 524 CZ2 TRP A 38152.669 10.492 -0.540 1.00 0.00 C ATOM 525 CZ3 TRP A 38152.256 8.216 -1.226 1.00 0.00 C ATOM 526 CH2 TRP A 38152.554 9.551 -1.526 1.00 0.00 C ATOM ATOM 527 H TRPA 38150.208 5.122 3.646 1.00 0.00 H

528 HA TRPA 38149.865 7.987 4.249 1.00 0.00 H ATOM 529 1HB TRP A 38152.215 7.565 4.310 1.00 0.00 H **ATOM** 530 2HB TRP A 38152.147 6.595 2.842 1.00 0.00 H **ATOM ATOM** 531 HD1 TRP A 38152.251 10.216 4.039 1.00 0.00 H 532 HE1 TRP A 38152.725 11.746 2.023 1.00 0.00 H ATOM 533 HE3 TRP A 38151.838 6.769 0.289 1.00 0.00 H **ATOM** 534 HZ2 TRP A 38152.896 11.518 -0.788 1.00 0.00 H ATOM 535 HZ3 TRP A 38152.173 7.503 -2.034 1.00 0.00 H **ATOM** 536 HH2 TRP A 38152.693 9.829 -2.560 1.00 0.00 H ATOM 537 N ILE A 39148.842 8.527 2.055 1.00 0.00 N **ATOM** 538 CA ILE A 39148.100 8.803 0.831 1.00 0.00 C **ATOM** 539 C ILEA 39148.544 10.127 0.223 1.00 0.00 C **ATOM ATOM** 540 O ILE A 39148.213 11.197 0.735 1.00 0.00 O 541 CB ILE A 39146.583 8.851 1.090 1.00 0.00 C **ATOM** 542 CG1 ILE A 39146.137 7.619 1.880 1.00 0.00 C ATOM 543 CG2 ILE A 39145.824 8.946 -0.225 1.00 0.00 C ATOM 544 CD1 ILE A 39144.728 7.725 2.420 1.00 0.00 C **ATOM** ATOM 545 H ILE A 39148.868 9.207 2.760 1.00 0.00 H ATOM: 546 HA ILE A 39148.302 8.007 0.129 1.00 0.00 H 547 HB ILE A 39146.366 9.737 1.667 1.00 0.00 H **ATOM** 548 1HG1 ILE A 39146.182 6.752 1.239 1.00 0.00 H ATOM 549 2HG1 ILE A 39146.804 7.476 2.717 1.00 0.00 H **ATOM** 550 1HG2 ILE A 39146.045 8.080 -0.832 1.00 0.00 H **ATOM** 551 2HG2 ILE A 39146.125 9.840 -0.752 1.00 0.00 H **ATOM** 552 3HG2 ILE A 39144.763 8.986 -0.028 1.00 0.00 H ATOM 553 1HD1 ILE A 39144.041 7.263 1.727 1.00 0.00 H **ATOM** 554 2HD1 ILE A 39144.468 8.765 2.547 1.00 0.00 H ATOM 555 3HD1 ILE A 39144.669 7.221 3.374 1.00 0.00 H ATOM 556 N GLYA 40149.303 10.051 -0.866 1.00 0.00 N ATOM 557 CA GLY A 40149.784 11.256 -1.513 1.00 0.00 C ATOM ATOM 558 C GLY A 40150.325 11.000 -2.905 1.00 0.00 C

559 O GLYA 40150.197 9.896 -3.437 1.00 0.00 O ATOM 560 H GLY A 40149.542 9.172 -1.228 1.00 0.00 H ATOM 561 1HA GLY A 40148.973 11.963 -1.580 1.00 0.00 H **ATOM** 562 2HA GLY A 40150.569 11.684 -0.909 1.00 0.00 H ATOM 563 N GLNA 41150.931 12.024 -3.494 1.00 0.00 N ATOM **ATOM** 564 CA GLN A 41151.497 11.918 -4.833 1.00 0.00 C 565 C GLN A 41152.964 12.346 -4.832 1.00 0.00 C ATOM **ATOM** 566 O GLN A 41153.276 13.509 -4.574 1.00 0.00 O 567 CB GLN A 41150.698 12.783 -5.807 1.00 0.00 C ATOM 568 CG GLN A 41149.196 12.573 -5.716 1.00 0.00 C **ATOM** 569 CD GLN A 41148.417 13.867 -5.845 1.00 0.00 C **ATOM** 570 OE1 GLN A 41148.369 14.671 -4.914 1.00 0.00 O ATOM 571 NE2 GLN A 41147.802 14.074 -7.002 1.00 0.00 N ATOM 572 H GLN A 41150.998 12.876 -3.016 1.00 0.00 H **ATOM** 573 HA GLN A 41151.430 10.886 -5.142 1.00 0.00 H ATOM 574 1HB GLN A 41150.906 13.822 -5.600 1.00 0.00 H ATOM 575 2HB GLN A 41151.013 12.556 -6.814 1.00 0.00 H **ATOM** 576 1HG GLN A 41148.889 11.906 -6.508 1.00 0.00 H ATOM 577 2HG GLN A 41148.965 12.125 -4.761 1.00 0.00 H **ATOM** 578 1HE2 GLN A 41147.884 13.389 -7.698 1.00 0.00 H **ATOM ATOM** 579 2HE2 GLN A 41147.291 14.902 -7.114 1.00 0.00 H 580 N PRO A 42153.889 11.412 -5.117 1.00 0.00 N **ATOM** 581 CA PRO A 42155.326 11.708 -5.142 1.00 0.00 C **ATOM** 582 C PRO A 42155.671 12.825 -6.122 1.00 0.00 C **ATOM** 583 O PRO A 42154.902 13.119 -7.038 1.00 0.00 O ATOM 584 CB PRO A 42155.961 10.387 -5.590 1.00 0.00 C **ATOM** 585 CG PRO A 42154.953 9.346 -5.249 1.00 0.00 C ATOM 586 CD PRO A 42153.614 10.000 -5.435 1.00 0.00 C **ATOM** 587 HA PRO A 42155.691 11.970 -4.160 1.00 0.00 H ATOM 588 1HB PRO A 42156.152 10.420 -6.653 1.00 0.00 H **ATOM** 589 2HB PRO A 42156.886 10.230 -5.057 1.00 0.00 H ATOM

590 1HG PRO A 42155.054 8.501 -5.913 1.00 0.00 H ATOM 591 2HG PRO A 42155.078 9.034 -4.222 1.00 0.00 H ATOM 592 1HD PRO A 42153,280 9.891 -6.457 1.00 0.00 H **ATOM ATOM** 593 2HD PRO A 42152.891 9.583 -4.751 1.00 0.00 H 594 N PRO A 43156.841 13.463 -5.943 1.00 0.00 N ATOM 595 CA PRO A 43157.286 14.551 -6.816 1.00 0.00 C ATOM 596 C PROA 43157.707 14.053 -8.193 1.00 0.00 C ATOM 597 O PROA 43158.879 13.762 -8.429 1.00 0.00 O ATOM 598 CB PRO A 43158.488 15.132 -6.072 1.00 0.00 C ATOM 599 CG PRO A 43159.013 14.001 -5.259 1.00 0.00 C **ATOM** 600 CD PRO A 43157.817 13.173 -4.876 1.00 0.00 C **ATOM** 601 HA PRO A 43156.525 15.310 -6.925 1.00 0.00 H **ATOM ATOM** 602 1HB PRO A 43159.220 15.481 -6.786 1.00 0.00 H 603 2HB PRO A 43158.167 15.952 -5.447 1.00 0.00 H ATOM 604 1HG PRO A 43159.702 13.414 -5.848 1.00 0.00 H ATOM 605 2HG PRO A 43159.504 14.381 -4.375 1.00 0.00 H ATOM ATOM 606 1HD PRO A 43158.074 12.124 -4.864 1.00 0.00 H ATOM 607 2HD PRO A 43157.438 13.479 -3.913 1.00 0.00 H 608 N GLY A 44156.742 13.956 -9.102 1.00 0.00 N ATOM 609 CA GLY A 44157.035 13.493 -10.444 1.00 0.00 C **ATOM** 610 C GLYA 44155.815 12.935 -11.146 1.00 0.00 C **ATOM** 611 O GLY A 44155.511 13.319 -12.275 1.00 0.00 O **ATOM** 612 H GLY A 44155.826 14.202 -8.859 1.00 0.00 H **ATOM ATOM** 613 1HA GLY A 44157.422 14.318 -11.021 1.00 0.00 H 614 2HA GLY A 44157.789 12.721 -10.389 1.00 0.00 H ATOM 615 N LEUA 45155.112 12.028 -10.476 1.00 0.00 N **ATOM** 616 CA LEU A 45153.916 11.419 -11.047 1.00 0.00 C ATOM 617 C LEUA 45152.704 11.673 -10.162 1.00 0.00 C **ATOM** 618 O LEUA 45152.622 11.161 -9.045 1.00 0.00 O ATOM 619 CB LEU A 45154.123 9.914 -11.228 1.00 0.00 C ATOM ATOM 620 CG LEU A 45154.702 9.190 -10.012 1.00 0.00 C

- ATOM 621 CD1 LEU A 45154.398 7.699 -10.079 1.00 0.00 C ATOM 622 CD2 LEU A 45156.202 9.431 -9.913 1.00 0.00 C
- ATOM 623 H LEU A 45155.402 11.763 -9.577 1.00 0.00 H
- ATOM 624 HA LEU A 45153.744 11.868 -12.013 1.00 0.00 H
- ATOM 625 1HB LEU A 45153.168 9.467 -11.467 1.00 0.00 H
- ATOM 626 2HB LEU A 45154.792 9.761 -12.061 1.00 0.00 H
- ATOM 627 HG LEU A 45154.240 9.583 -9.116 1.00 0.00 H
- ATOM 628 1HD1 LEU A 45153.895 7.394 -9.174 1.00 0.00 H
- ATOM 629 2HD1 LEU A 45155.321 7.147 -10.182 1.00 0.00 H
- ATOM 630 3HD1 LEU A 45153.763 7.498 -10.930 1.00 0.00 H
- ATOM 631 1HD2 LEU A 45156.405 10.107 -9.095 1.00 0.00 H
- ATOM 632 2HD2 LEU A 45156.558 9.867 -10.836 1.00 0.00 H
- ATOM 633 3HD2 LEU A 45156.709 8.493 -9.739 1.00 0.00 H
- ATOM 634 N ASN A 46151.760 12.464 -10.662 1.00 0.00 N
- ATOM 635 CA ASN A 46150.556 12.771 -9.903 1.00 0.00 C
- ATOM 636 C ASN A 46149.628 11.563 -9.860 1.00 0.00 C
- ATOM 637 O ASN A 46149.007 11.207 -10.861 1.00 0.00 O
- ATOM 638 CB ASN A 46149.829 13.967 -10.521 1.00 0.00 C
- ATOM 639 CG ASN A 46148.973 14.709 -9.514 1.00 0.00 C
- ATOM 640 OD1 ASN A 46147.746 14.622 -9.540 1.00 0.00 O
- ATOM 641 ND2 ASN A 46149.619 15.445 -8.617 1.00 0.00 N
- ATOM 642 H ASN A 46151.875 12.844 -11.558 1.00 0.00 H
- ATOM 643 HA ASN A 46150.852 13.021 -8.895 1.00 0.00 H
- ATOM 644 1HB ASN A 46150.557 14.655 -10.922 1.00 0.00 H
- ATOM 645 2HB ASN A 46149.191 13.619 -11.320 1.00 0.00 H
- ATOM 646 1HD2 ASN A 46150.599 15.468 -8.655 1.00 0.00 H
- ATOM 647 2HD2 ASN A 46149.091 15.936 -7.953 1.00 0.00 H
- ATOM 648 N GLUA 47149.543 10.935 -8.693 1.00 0.00 N
- ATOM 649 CA GLU A 47148.693 9.766 -8.511 1.00 0.00 C
- ATOM 650 C GLU A 47148.523 9.444 -7.031 1.00 0.00 C
- ATOM 651 O GLU A 47149.502 9.193 -6.327 1.00 0.00 O

- ATOM 652 CB GLU A 47149.286 8.558 -9.243 1.00 0.00 C
- ATOM 653 CG GLU A 47150.801 8.468 -9.150 1.00 0.00 C
- ATOM 654 CD GLU A 47151.389 7.499 -10.156 1.00 0.00 C
- ATOM 655 OE1 GLU A 47151.498 7.871 -11.345 1.00 0.00 O
- ATOM 656 OE2 GLU A 47151.742 6.370 -9.757 1.00 0.00 O
- ATOM 657 H GLUA 47150.064 11.268 -7.933 1.00 0.00 H
- ATOM 658 HA GLU A 47147.725 9.991 -8.932 1.00 0.00 H
- ATOM 659 1HB GLU A 47148.866 7.656 -8.820 1.00 0.00 H
- ATOM 660 2HB GLU A 47149.014 8.615 -10.286 1.00 0.00 H
- ATOM 661 1HG GLU A 47151.218 9.446 -9.329 1.00 0.00 H
- ATOM 662 2HG GLU A 47151.070 8.140 -8.157 1.00 0.00 H
- ATOM 663 N VALA 48147.281 9.445 -6.564 1.00 0.00 N
- ATOM 664 CA VALA 48146.998 9.146 -5.167 1.00 0.00 C
- ATOM 665 C VALA 48147.382 7.708 -4.839 1.00 0.00 C
- ATOM 666 O VALA 48146.654 6.771 -5.164 1.00 0.00 O
- ATOM 667 CB VAL A 48145.510 9.358 -4.832 1.00 0.00 C
- ATOM 668 CG1 VAL A 48145.280 9.261 -3.332 1.00 0.00 C
- ATOM 669 CG2 VAL A 48145.028 10.698 -5.367 1.00 0.00 C
- ATOM 670 H VALA 48146.539 9.647 -7.171 1.00 0.00 H
- ATOM 671 HA VAL A 48147.586 9.814 -4.555 1.00 0.00 H
- ATOM 672 HB VALA 48144.938 8.577 -5.311 1.00 0.00 H
- ATOM 673 1HG1 VAL A 48146.009 9.870 -2.816 1.00 0.00 H
- ATOM 674 2HG1 VAL A 48145.384 8.234 -3.018 1.00 0.00 H
- ATOM 675 3HG1 VAL A 48144.286 9.612 -3.096 1.00 0.00 H
- ATOM 676 1HG2 VAL A 48144.888 10.631 -6.435 1.00 0.00 H
- ATOM 677 2HG2 VAL A 48145.764 11.458 -5.149 1.00 0.00 H
- ATOM 678 3HG2 VAL A 48144.092 10.958 -4.896 1.00 0.00 H
- ATOM 679 N LEU A 49148.535 7.539 -4.201 1.00 0.00 N
- ATOM 680 CA LEUA 49149.018 6.214 -3.836 1.00 0.00 C
- ATOM 681 C LEUA 49148.878 5.981 -2.338 1.00 0.00 C
- ATOM 682 O LEUA 49149.538 6.638 -1.532 1.00 0.00 O

683 CB LEU A 49150.480 6.046 -4.256 1.00 0.00 C **ATOM** 684 CG LEU A 49150.733 6.129 -5.763 1.00 0.00 C ATOM 685 CD1 LEU A 49152.125 6.676 -6.041 1.00 0.00 C **ATOM** 686 CD2 LEU A 49150.556 4.763 -6.408 1.00 0.00 C ATOM ATOM 687 H LEUA 49149.075 8.325 -3.971 1.00 0.00 H **ATOM** 688 HA LEU A 49148.417 5.486 -4.360 1.00 0.00 H 689 1HB LEU A 49151.062 6.815 -3.771 1.00 0.00 H ATOM 690 2HB LEU A 49150.824 5.084 -3.910 1.00 0.00 H **ATOM** 691 HG LEU A 49150.016 6.805 -6.206 1.00 0.00 H **ATOM** 692 1HD1 LEU A 49152.859 6.065 -5.535 1.00 0.00 H ATOM 693 2HD1 LEU A 49152.192 7.691 -5.679 1.00 0.00 H ATOM 694 3HD1 LEU A 49152.313 6.658 -7.104 1.00 0.00 H ATOM 695 1HD2 LEU A 49151.466 4.192 -6.299 1.00 0.00 H ATOM 696 2HD2 LEU A 49150.332 4.887 -7.458 1.00 0.00 H **ATOM ATOM** 697 3HD2 LEU A 49149.744 4.241 -5.927 1.00 0.00 H 698 N ALAA 50148.016 5.041 -1.969 1.00 0.00 N **ATOM ATOM** -699 CA ALAA 50147.792 4.725 -0.567 1.00 0.00 C 700 C ALAA 50148.710 3.597 -0.106 1.00 0.00 C ATOM 701 O ALAA 50148.601 2.465 -0.577 1.00 0.00 O ATOM **ATOM** 702 CB ALAA 50146.334 4.353 -0.335 1.00 0.00 C 703 H ALAA 50147.518 4.551 -2.657 1.00 0.00 H **ATOM ATOM** 704 HA ALA A 50148.009 5.613 0.009 1.00 0.00 H 705 1HB ALA A 50145.791 5.222 0.005 1.00 0.00 H **ATOM** 706 2HB ALA A 50146.275 3.576 0.412 1.00 0.00 H ATOM 707 3HB ALA A 50145.903 3.997 -1.259 1.00 0.00 H **ATOM** 708 N GLYA 51149.612 3.914 0.815 1.00 0.00 N **ATOM** 709 CA GLY A 51150.535 2.916 1.323 1.00 0.00 C **ATOM** 710 C GLYA 51149.844 1.863 2.167 1.00 0.00 C **ATOM** 711 O GLY A 51149.329 2.161 3.245 1.00 0.00 O **ATOM ATOM** 712 H GLY A 51149.653 4.833 1.153 1.00 0.00 H 713 1HA GLY A 51151.018 2.431 0.488 1.00 0.00 H ATOM

714 2HA GLY A 51151.286 3.408 1.924 1.00 0.00 H **ATOM** 715 N LEUA 52149.831 0.629 1.676 1.00 0.00 N ATOM 716 CA LEU A 52149.197 -0.472 2.394 1.00 0.00 C **ATOM ATOM** 717 C LEU A 52150.243 -1.373 3.043 1.00 0.00 C 718 O LEUA 52151.202 -1.795 2.395 1.00 0.00 O ATOM **ATOM** 719 CB LEU A 52148.321 -1.291 1.444 1.00 0.00 C 720 CG LEU A 52147.056 -0.582 0.958 1.00 0.00 C ATOM **ATOM** 721 CD1 LEU A 52146.413 -1.358 -0.180 1.00 0.00 C **ATOM** 722 CD2 LEU A 52146.072 -0.402 2.105 1.00 0.00 C 723 H LEUA 52150.258 0.452 0.813 1.00 0.00 H **ATOM** 724 HA LEUA 52148.576 -0.048 3.168 1.00 0.00 H **ATOM** 725 1HB LEU A 52148.914 -1.558 0.582 1.00 0.00 H ATOM ATOM 726 2HB LEU A 52148.025 -2.197 1.951 1.00 0.00 H ATOM 727 HG LEU A 52147.320 0.398 0.587 1.00 0.00 H 728 1HD1 LEU A 52147.183 -1.760 -0.823 1.00 0.00 H ATOM **ATOM** 729 2HD1 LEU A 52145.776 -0.698 -0.752 1.00 0.00 H **ATOM** 730 3HD1 LEU A 52145.822 -2.167 0.223 1.00 0.00 H 731 1HD2 LEU A 52146.235 -1.174 2.843 1.00 0.00 H ATOM 732 2HD2 LEU A 52145.063 -0.473 1.728 1.00 0.00 H **ATOM** ATOM 733 3HD2 LEU A 52146.220 0.567 2.558 1.00 0.00 H 734 N GLUA 53150.052 -1.664 4.326 1.00 0.00 N **ATOM** 735 CA GLUA 53150.978 -2.514 5.063 1.00 0.00 C **ATOM** 736 C GLUA 53150.455 -3.945 5.146 1.00 0.00 C **ATOM** 737 O GLUA 53149.489 -4.223 5.858 1.00 0.00 O **ATOM** 738 CB GLU A 53151.204 -1.959 6.470 1.00 0.00 C ATOM 739 CG GLU A 53152.193 -2.769 7.292 1.00 0.00 C ATOM 740 CD GLUA 53151.825 -2.820 8.762 1.00 0.00 C ATOM 741 OE1 GLU A 53150.789 -3.436 9.095 1.00 0.00 O ATOM 742 OE2 GLU A 53152.571 -2.244 9.581 1.00 0.00 O ATOM **ATOM** 743 H GLUA 53149.269 -1.297 4.787 1.00 0.00 H 744 HA GLU A 53151.919 -2.519 4.532 1.00 0.00 H ATOM

745 1HB GLUA 53151.577 -0.949 6.391 1.00 0.00 H **ATOM** 746 2HB GLU A 53150.259 -1.944 6.995 1.00 0.00 H ATOM **ATOM** 747 1HG GLU A 53152.219 -3.779 6.909 1.00 0.00 H **ATOM** 748 2HG GLU A 53153.172 -2.323 7.196 1.00 0.00 H 749 N LEUA 54151.097 -4.848 4.413 1.00 0.00 N ATOM 750 CA LEU A 54150.696 -6.250 4.404 1.00 0.00 C **ATOM** 751 C LEUA 54150.964 -6.903 5.757 1.00 0.00 C ATOM 752 O LEUA 54152.037 -6.735 6.335 1.00 0.00 O **ATOM** 753 CB LEU A 54151.439 -7.008 3.302 1.00 0.00 C **ATOM** 754 CG LEUA 54151.377 -6.362 1.917 1.00 0.00 C **ATOM** 755 CD1 LEU A 54152.577 -6.778 1.080 1.00 0.00 C **ATOM** 756 CD2 LEU A 54150.080 -6.734 1.215 1.00 0.00 C ATOM **ATOM** 757 H LEUA 54151.859 -4.565 3.866 1.00 0.00 H 758 HA LEUA 54149.635 -6.290 4.203 1.00 0.00 H ATOM 759 1HB LEU A 54152.476 -7.094 3.591 1.00 0.00 H **ATOM** 760 2HB LEUA 54151.019 -8.000 3.231 1.00 0.00 H **ATOM** 761 HG LEUA 54151.404 -5.288 2.026 1.00 0.00 H **ATOM** 762 1HD1 LEU A 54152.294 -6.815 0.038 1.00 0.00 H **ATOM ATOM** 763 2HD1 LEU A 54152.914 -7.755 1.396 1.00 0.00 H 764 3HD1 LEU A 54153.373 -6.062 1.212 1.00 0.00 H ATOM 765 1HD2 LEU A 54150.087 -6.336 0.212 1.00 0.00 H **ATOM** 766 2HD2 LEU A 54149.244 -6.321 1.761 1.00 0.00 H ATOM 767 3HD2 LEU A 54149.988 -7.809 1.175 1.00 0.00 H **ATOM ATOM** 768 N GLUA 55149.981 -7.645 6.255 1.00 0.00 N 769 CA GLUA 55150.112 -8.323 7.540 1.00 0.00 C **ATOM** 770 C GLUA 55151.134 -9.452 7.459 1.00 0.00 C **ATOM** 771 O GLUA 55151.849 -9.725 8.422 1.00 0.00 O **ATOM** 772 CB GLU A 55148.758 -8.876 7.988 1.00 0.00 C **ATOM ATOM** 773 CG GLUA 55147.661 -7.825 8.049 1.00 0.00 C 774 CD GLUA 55146.606 -8.144 9.089 1.00 0.00 C **ATOM** 775 OE1 GLU A 55146.111 -7.202 9.743 1.00 0.00 O ATOM

776 OE2 GLU A 55146.273 -9.338 9.250 1.00 0.00 O ATOM 777 H GLUA 55149.149 -7.740 5.746 1.00 0.00 H **ATOM** 778 HA GLU A 55150.452 -7.597 8.264 1.00 0.00 H **ATOM ATOM** 779 1HB GLU A 55148.450 -9.646 7.297 1.00 0.00 H ATOM 780 2HB GLU A 55148.867 -9.310 8.971 1.00 0.00 H 781 1HG GLU A 55148.106 -6.873 8.292 1.00 0.00 H **ATOM** 782 2HG GLU A 55147.185 -7.764 7.081 1.00 0.00 H ATOM 783 N ASPA 56151.196 -10.104 6.302 1.00 0.00 N **ATOM** 784 CA ASP A 56152.131 -11.204 6.095 1.00 0.00 C ATOM **ATOM** 785 C ASPA 56153.441 -10.699 5.500 1.00 0.00 C 786 O ASPA 56153.443 -9.875 4.585 1.00 0.00 O **ATOM** 787 CB ASP A 56151.513 -12.260 5.178 1.00 0.00 C **ATOM ATOM** 788 CG ASP A 56151.896 -13.671 5.579 1.00 0.00 C 789 OD1 ASP A 56152.482 -14.388 4.741 1.00 0.00 O ATOM **ATOM** 790 OD2 ASP A 56151.612 -14.057 6.733 1.00 0.00 O 791 H ASPA 56150.601 -9.839 5.571 1.00 0.00 H ATOM 792 HA ASP A 56152.336 -11.650 7.057 1.00 0.00 H **ATOM** ATOM 793 1HB ASP A 56150.437 -12.175 5.214 1.00 0.00 H **ATOM** 794 2HB ASP A 56151.849 -12.090 4.165 1.00 0.00 H 795 N GLUA 57154.555 -11.200 6.023 1.00 0.00 N ATOM 796 CA GLU A 57155.873 -10.799 5.543 1.00 0.00 C **ATOM** 797 C GLUA 57156.191 -11.467 4.209 1.00 0.00 C ATOM 798 O GLUA 57156.569 -12.637 4.163 1.00 0.00 O ATOM **ATOM** 799 CB GLU A 57156.945 -11.158 6.573 1.00 0.00 C 800 CG GLU A 57157.202 -10.058 7.591 1.00 0.00 C ATOM 801 CD GLU A 57158.675 -9.895 7.913 1.00 0.00 C ATOM 802 OE1 GLU A 57159.507 -10.090 7.002 1.00 0.00 O ATOM 803 OE2 GLU A 57158.996 -9.573 9.076 1.00 0.00 O ATOM 804 H GLU A 57154.490 -11.854 6.750 1.00 0.00 H ATOM 805 HA GLUA 57155.864 -9.729 5.403 1.00 0.00 H ATOM ATOM 806 1HB GLU A 57156.635 -12.045 7.106 1.00 0.00 H

- ATOM 807 2HB GLU A 57157.871 -11.364 6.057 1.00 0.00 H
- ATOM 808 1HG GLU A 57156.832 -9.125 7.194 1.00 0.00 H
- ATOM 809 2HG GLU A 57156.673 -10.298 8.502 1.00 0.00 H
- ATOM 810 N CYS A 58156.035 -10.715 3.125 1.00 0.00 N
- ATOM 811 CA CYS A 58156.305 -11.234 1.789 1.00 0.00 C
- ATOM 812 C CYS A 58157.612 -10.668 1.241 1.00 0.00 C
- ATOM 813 O CYS A 58157.877 -9.472 1.350 1.00 0.00 O
- ATOM 814 CB CYS A 58155.153 -10.892 0.844 1.00 0.00 C
- ATOM 815 SG CYS A 58154.828 -12.155 -0.409 1.00 0.00 S
- ATOM 816 H CYS A 58155.731 -9.788 3.225 1.00 0.00 H
- ATOM 817 HA CYS A 58156.393 -12.307 1.862 1.00 0.00 H
- ATOM 818 1HB CYS A 58154.249 -10.764 1.421 1.00 0.00 H
- ATOM 819 2HB CYS A 58155.378 -9.970 0.330 1.00 0.00 H
- ATOM 820 HG CYS A 58155.382 -11.967 -1.171 1.00 0.00 H
- ATOM 821 N ALA A 59158.424 -11.538 0.649 1.00 0.00 N
- ATOM 822 CA ALA A 59159.704 -11.127 0.083 1.00 0.00 C
- ATOM 823 C ALA A 59159.504 -10.336 -1.206 1.00 0.00 C
- ATOM 824 O ALA A 59158.946 -10.845 -2.177 1.00 0.00 O
- ATOM 825 CB ALA A 59160.583 -12.342 -0.172 1.00 0.00 C
- ATOM 826 H ALA A 59158.157 -12.480 0.592 1.00 0.00 H
- ATOM 827 HA ALA A 59160.201 -10.498 0.806 1.00 0.00 H
- ATOM 828 1HB ALA A 59160.533 -13.006 0.679 1.00 0.00 H
- ATOM 829 2HB ALA A 59161.604 -12.022 -0.319 1.00 0.00 H
- ATOM 830 3HB ALA A 59160.235 -12.859 -1.053 1.00 0.00 H
- ATOM 831 N GLY A 60159.964 -9.090 -1.206 1.00 0.00 N
- ATOM 832 CA GLY A 60159.828 -8.249 -2.381 1.00 0.00 C
- ATOM 833 C GLY A 60159.332 -6.857 -2.044 1.00 0.00 C
- ATOM 834 O GLY A 60159.634 -5.895 -2.751 1.00 0.00 O
- ATOM 835 H GLY A 60160.402 -8.738 -0.403 1.00 0.00 H
- ATOM 836 1HA GLY A 60160.789 -8.169 -2.868 1.00 0.00 H
- ATOM 837 2HA GLY A 60159.129 -8.713 -3.063 1.00 0.00 H

- ATOM 838 N CYS A 61158.569 -6.749 -0.961 1.00 0.00 N
- ATOM 839 CA CYS A 61158.030 -5.464 -0.533 1.00 0.00 C
- ATOM 840 C CYS A 61159.088 -4.647 0.201 1.00 0.00 C
- ATOM 841 O CYS A 61160.199 -5.122 0.439 1.00 0.00 O
- ATOM 842 CB CYS A 61156.814 -5.674 0.372 1.00 0.00 C
- ATOM 843 SG CYS A 61155.538 -6.739 -0.343 1.00 0.00 S
- ATOM 844 H CYS A 61158.363 -7.552 -0.440 1.00 0.00 H
- ATOM 845 HA CYS A 61157.721 -4.923 -1.414 1.00 0.00 H
- ATOM 846 1HB CYS A 61157.137 -6.126 1.297 1.00 0.00 H
- ATOM 847 2HB CYS A 61156.361 -4.716 0.584 1.00 0.00 H
- ATOM 848 HG CYS A 61155.374 -6.443 -1.241 1.00 0.00 H
- ATOM 849 N THR A 62158.736 -3.416 0.557 1.00 0.00 N
- ATOM 850 CA THR A 62159.656 -2.532 1.265 1.00 0.00 C
- ATOM 851 C THR A 62159.205 -2.320 2.707 1.00 0.00 C
- ATOM 852 O THR A 62158.208 -2.893 3.147 1.00 0.00 O
- ATOM 853 CB THR A 62159.755 -1.186 0.546 1.00 0.00 C
- ATOM 854 OG1 THR A 62158.468 -0.633 0.336 1.00 0.00 O
- ATOM 855 CG2 THR A 62160.441 -1.276 -0.800 1.00 0.00 C
- ATOM 856 H THR A 62157.835 -3.094 0.341 1.00 0.00 H
- ATOM 857 HA THR A 62160.628 -3.001 1.270 1.00 0.00 H
- ATOM 858 HB THR A 62160.322 -0.502 1.161 1.00 0.00 H
- ATOM 859 HG1 THR A 62158.158 -0.226 1.149 1.00 0.00 H
- ATOM 860 1HG2 THR A 62160.407 -2.296 -1.154 1.00 0.00 H
- ATOM 861 2HG2 THR A 62161.470 -0.963 -0.701 1.00 0.00 H
- ATOM 862 3HG2 THR A 62159.936 -0.634 -1.506 1.00 0.00 H
- ATOM 863 N ASPA 63159.946 -1.492 3.437 1.00 0.00 N
- ATOM 864 CA ASPA 63159.622 -1.204 4.830 1.00 0.00 C
- ATOM 865 C ASP A 63158.872 0.118 4.951 1.00 0.00 C
- ATOM 866 O ASPA 63158.994 0.823 5.953 1.00 0.00 O
- ATOM 867 CB ASPA 63160.897 -1.160 5.673 1.00 0.00 C
- ATOM 868 CG ASP A 63161.958 -0.260 5.071 1.00 0.00 C

ATOM 869 OD1 ASP A 63161.917 0.962 5.329 1.00 0.00 O 870 OD2 ASP A 63162.830 -0.775 4.341 1.00 0.00 O **ATOM** 871 H ASPA 63160.728 -1.066 3.030 1.00 0.00 H **ATOM** 872 HA ASPA 63158.988 -1.998 5.194 1.00 0.00 H ATOM ATOM 873 1HB ASP A 63160.658 -0.792 6.659 1.00 0.00 H ATOM 874 2HB ASPA 63161.302 -2.158 5.755 1.00 0.00 H 875 N GLY A 64158.097 0.449 3.923 1.00 0.00 N **ATOM ATOM** 876 CA GLY A 64157.338 1.687 3.936 1.00 0.00 C **ATOM** 877 C GLY A 64158.086 2.832 3.282 1.00 0.00 C 878 O GLY A 64158.057 3.960 3.772 1.00 0.00 O **ATOM** 879 H GLY A 64158.038 -0.151 3.152 1.00 0.00 H **ATOM** 880 1HA GLY A 64156.408 1.532 3.409 1.00 0.00 H ATOM ATOM 881 2HA GLY A 64157.119 1.951 4.959 1.00 0.00 H **ATOM** 882 N THR A 65158.759 2.540 2.173 1.00 0.00 N **ATOM** 883 CA THR A 65159.518 3.555 1.451 1.00 0.00 C 884 C THR A 65159.186 3.527 -0.037 1.00 0.00 C **ATOM ATOM** 885 O THR A 65159.401 2.520 -0.712 1.00 0.00 O ATOM 886 CB THR A 65161.018 3.339 1.654 1.00 0.00 C 887 OG1 THR A 65161.361 1.979 1.450 1.00 0.00 O **ATOM ATOM** 888 CG2 THR A 65161.498 3.730 3.036 1.00 0.00 C 889 H THR A 65158.743 1.622 1.832 1.00 0.00 H **ATOM** 890 HA THR A 65159.246 4.520 1.851 1.00 0.00 H **ATOM** 891 HB THR A 65161.559 3.937 0.935 1.00 0.00 H **ATOM** 892 HG1 THR A 65160.987 1.675 0.620 1.00 0.00 H **ATOM** 893 1HG2 THR A 65161.971 2.882 3.507 1.00 0.00 H ATOM 894 2HG2 THR A 65160.656 4.050 3.632 1.00 0.00 H **ATOM ATOM** 895 3HG2 THR A 65162.209 4.539 2.954 1.00 0.00 H 896 N PHE A 66158.661 4.639 -0.541 1.00 0.00 N **ATOM** 897 CA PHE A 66158.299 4.742 -1.950 1.00 0.00 C **ATOM ATOM** 898 C PHE A 66159.221 5.716 -2.679 1.00 0.00 C 899 O PHE A 66159.301 6.892 -2.326 1.00 0.00 O ATOM

900 CB PHE A 66156.845 5.196 -2.093 1.00 0.00 C **ATOM** 901 CG PHE A 66156.255 4.906 -3.443 1.00 0.00 C ATOM 902 CD1 PHE A 66155.891 3.615 -3.791 1.00 0.00 C **ATOM ATOM** 903 CD2 PHE A 66156.065 5.924 -4.364 1.00 0.00 C **ATOM** 904 CE1 PHE A 66155.348 3.345 -5.033 1.00 0.00 C **ATOM** 905 CE2 PHE A 66155.523 5.659 -5.607 1.00 0.00 C ATOM 906 CZ PHE A 66155.163 4.368 -5.943 1.00 0.00 C 907 H PHE A 66158.514 5.408 0.047 1.00 0.00 H **ATOM** 908 HA PHE A 66158.406 3.764 -2.393 1.00 0.00 H ATOM **ATOM** 909 1HB PHE A 66156.243 4.691 -1.353 1.00 0.00 H 910 2HB PHE A 66156.791 6.263 -1.927 1.00 0.00 H ATOM 911 HD1 PHE A 66156.035 2.814 -3.082 1.00 0.00 H ATOM 912 HD2 PHE A 66156.345 6.933 -4.104 1.00 0.00 H **ATOM** 913 HE1 PHE A 66155.069 2.333 -5.293 1.00 0.00 H ATOM **ATOM** 914 HE2 PHE A 66155.379 6.461 -6.316 1.00 0.00 H ATOM 915 HZ PHE A 66154.739 4.159 -6.913 1.00 0.00 H 916 N ARG A 67159.915 5.216 -3.697 1.00 0.00 N **ATOM** ATOM 917 CA ARG A 67160.832 6.041 -4.475 1.00 0.00 C **ATOM** 918 C ARGA 67161.929 6.620 -3.587 1.00 0.00 C **ATOM** 919 O ARGA 67162.433 7.715 -3.841 1.00 0.00 O 920 CB ARG A 67160.070 7.173 -5.166 1.00 0.00 C ATOM 921 CG ARG A 67158.877 6.694 -5.979 1.00 0.00 C **ATOM** 922 CD ARG A 67159.187 6.672 -7.467 1.00 0.00 C **ATOM ATOM** 923 NE ARG A 67158.148 5.989 -8.234 1.00 0.00 N 924 CZ ARG A 67158.009 6.095 -9.553 1.00 0.00 C **ATOM ATOM** 925 NH1 ARG A 67158.840 6.854 -10.257 1.00 0.00 N 926 NH2 ARG A 67157.035 5.440 -10.172 1.00 0.00 N **ATOM** 927 H ARGA 67159.809 4.270 -3.929 1.00 0.00 H **ATOM** ATOM 928 HA ARG A 67161.287 5.413 -5.225 1.00 0.00 H 929 1HB ARG A 67159.713 7.862 -4.417 1.00 0.00 H **ATOM** 930 2HB ARG A 67160.746 7.692 -5.830 1.00 0.00 H

931 1HG ARG A 67158.615 5.696 -5.662 1.00 0.00 H 932 2HG ARG A 67158.045 7.361 -5.805 1.00 0.00 H **ATOM** 933 1HD ARG A 67159.272 7.689 -7.821 1.00 0.00 H **ATOM ATOM** 934 2HD ARG A 67160.127 6.161 -7.618 1.00 0.00 H 935 HE ARG A 67157.520 5.422 -7.739 1.00 0.00 H ATOM 936 1HH1 ARG A 67159.576 7.350 -9.797 1.00 0.00 H ATOM 937 2HH1 ARG A 67158.731 6.929 -11.248 1.00 0.00 H ATOM 938 1HH2 ARG A 67156.407 4.867 -9.647 1.00 0.00 H ATOM 939 2HH2 ARG A 67156.931 5.520 -11.163 1.00 0.00 H **ATOM** 940 N GLYA 68162.294 5.880 -2.546 1.00 0.00 N ATOM 941 CA GLY A 68163.328 6.336 -1.637 1.00 0.00 C **ATOM** 942 C GLYA 68162.851 7.452 -0.728 1.00 0.00 C **ATOM** 943 O GLY A 68163.645 8.277 -0.277 1.00 0.00 O ATOM 944 H GLYA 68161.858 5.016 -2.394 1.00 0.00 H **ATOM** ATOM 945 1HA GLY A 68163.650 5.504 -1.028 1.00 0.00 H 946 2HA GLY A 68164.169 6.692 -2.215 1.00 0.00 H ATOM ATOM 947 N THR A 69161.549 7.477 -0.459 1.00 0.00 N 948 CA THR A 69160.967 8.500 0.402 1.00 0.00 C ATOM 949 C THR A 69160.013 7.879 1.417 1.00 0.00 C **ATOM** 950 O THR A 69158.835 7.665 1.126 1.00 0.00 O ATOM **ATOM** 951 CB THR A 69160.228 9.543 -0.438 1.00 0.00 C 952 OG1 THR A 69161.060 10.033 -1.474 1.00 0.00 O ATOM 953 CG2 THR A 69159.750 10.732 0.367 1.00 0.00 C **ATOM** 954 H THR A 69160.967 6.792 -0.848 1.00 0.00 H ATOM 955 HA THR A 69161.772 8.984 0.934 1.00 0.00 H ATOM 956 HB THR A 69159.362 9.079 -0.889 1.00 0.00 H ATOM 957 HG1 THR A 69161.864 10.397 -1.095 1.00 0.00 H **ATOM** 958 1HG2 THR A 69158.755 11.006 0.048 1.00 0.00 H **ATOM** 959 2HG2 THR A 69160.421 11.564 0.214 1.00 0.00 H ATOM 960 3HG2 THR A 69159.732 10.473 1.416 1.00 0.00 H **ATOM** ATOM 961 N ARG A 70160.528 7.590 2.608 1.00 0.00 N

962 CA ARG A 70159.721 6.993 3.665 1.00 0.00 C ATOM ATOM 963 C ARGA 70158.604 7.938 4.097 1.00 0.00 C **ATOM** 964 O ARGA 70158.855 9.085 4.463 1.00 0.00 O ATOM 965 CB ARG A 70160.598 6.640 4.867 1.00 0.00 C 966 CG ARG A 70159.836 5.977 6.004 1.00 0.00 C ATOM ATOM 967 CD ARG A 70160.300 6.481 7.361 1.00 0.00 C **ATOM** 968 NE ARG A 70160.874 5.412 8.175 1.00 0.00 N ATOM 969 CZ ARG A 70161.488 5.614 9.338 1.00 0.00 C **ATOM** 970 NH1 ARG A 70161.607 6.842 9.829 1.00 0.00 N **ATOM** 971 NH2 ARG A 70161.982 4.586 10.014 1.00 0.00 N ATOM 972 H ARGA 70161.472 7.783 2.779 1.00 0.00 H ATOM 973 HA ARG A 70159.279 6.088 3.274 1.00 0.00 H ATOM 974 1HB ARG A 70161.378 5.965 4.544 1.00 0.00 H **ATOM** 975 2HB ARG A 70161.052 7.544 5.245 1.00 0.00 H 976 1HG ARG A 70158.784 6.193 5.892 1.00 0.00 H ATOM 977 2HG ARG A 70159.992 4.908 5.953 1.00 0.00 H **ATOM** 978 1HD ARG A 70161.046 7.247 7.213 1.00 0.00 H ATOM 979 2HD ARG A 70159.453 6.901 7.883 1.00 0.00 H ATOM 980 HE ARG A 70160.800 4.496 7.836 1.00 0.00 H ATOM 981 1HH1 ARG A 70161.237 7.621 9.325 1.00 0.00 H ATOM 982 2HH1 ARG A 70162.069 6.987 10.705 1.00 0.00 H ATOM ATOM 983 1HH2 ARG A 70161.894 3.659 9.650 1.00 0.00 H 984 2HH2 ARG A 70162.443 4.738 10.889 1.00 0.00 H ATOM **ATOM** 985 N TYR A 71157.370 7.446 4.052 1.00 0.00 N 986 CA TYR A 71156.214 8.246 4.439 1.00 0.00 C ATOM ATOM 987 C TYR A 71155.763 7.901 5.855 1.00 0.00 C 988 O TYRA 71155.335 8.772 6.611 1.00 0.00 O **ATOM** 989 CB TYR A 71155.062 8.026 3.457 1.00 0.00 C ATOM 990 CG TYR A 71155.320 8.599 2.082 1.00 0.00 C **ATOM** 991 CD1 TYR A 71155.325 7.783 0.958 1.00 0.00 C ATOM 992 CD2 TYR A 71155.557 9.957 1.908 1.00 0.00 C

993 CE1 TYR A 71155.560 8.303 -0.301 1.00 0.00 C 994 CE2 TYR A 71155.793 10.485 0.652 1.00 0.00 C ATOM 995 CZ TYR A 71155.794 9.654 -0.448 1.00 0.00 C ATOM 996 OH TYR A 71156.028 10.176 -1.700 1.00 0.00 O ATOM 997 H TYR A 71157.233 6.523 3.751 1.00 0.00 H ATOM ATOM 998 HA TYR A 71156.506 9.285 4.410 1.00 0.00 H 999 1HB TYR A 71154.891 6.965 3.347 1.00 0.00 H ATOM ATOM 1000 2HB TYR A 71154.170 8.491 3.849 1.00 0.00 H ATOM 1001 HD1 TYR A 71155.142 6.725 1.076 1.00 0.00 H ATOM 1002 HD2 TYR A 71155.557 10.605 2.772 1.00 0.00 H ATOM 1003 HE1 TYR A 71155.561 7.653 -1.163 1.00 0.00 H ATOM 1004 HE2 TYR A 71155.976 11.543 0.538 1.00 0.00 H ATOM 1005 HH TYR A 71155.312 9.928 -2.289 1.00 0.00 H ATOM 1006 N PHE A 72155.865 6.623 6.207 1.00 0.00 N ATOM 1007 CA PHE A 72155.467 6.162 7.533 1.00 0.00 C ATOM 1008 C PHE A 72156.458 5.134 8.069 1.00 0.00 C ATOM 1009 O PHE A 72157.415 4.764 7.388 1.00 0.00 O ATOM 1010 CB PHE A 72154.063 5.558 7.486 1.00 0.00 C ATOM 1011 CG PHE A 72153.887 4.530 6.405 1.00 0.00 C ATOM 1012 CD1 PHE A 72153.603 4.914 5.104 1.00 0.00 C ATOM 1013 CD2 PHE A 72154.006 3.179 6.690 1.00 0.00 C ATOM 1014 CE1 PHE A 72153.441 3.971 4.108 1.00 0.00 C ATOM 1015 CE2 PHE A 72153.844 2.231 5.697 1.00 0.00 C ATOM 1016 CZ PHE A 72153.562 2.628 4.405 1.00 0.00 C ATOM 1017 H PHE A 72156.214 5.975 5.561 1.00 0.00 H ATOM 1018 HA PHE A 72155.461 7.017 8.192 1.00 0.00 H ATOM 1019 1HB PHE A 72153.851 5.084 8.432 1.00 0.00 H ATOM 1020 2HB PHE A 72153.345 6.348 7.315 1.00 0.00 H ATOM 1021 HD1 PHE A 72153.509 5.965 4.871 1.00 0.00 H ATOM 1022 HD2 PHE A 72154.227 2.868 7.700 1.00 0.00 H ATOM 1023 HE1 PHE A 72153.219 4.284 3.097 1.00 0.00 H

ATOM 1024 HE2 PHE A 72153.939 1.181 5.932 1.00 0.00 H ATOM 1025 HZ PHE A 72153.435 1.888 3.628 1.00 0.00 H ATOM 1026 N THR A 73156.221 4.676 9.294 1.00 0.00 N ATOM 1027 CA THR A 73157.093 3.690 9.923 1.00 0.00 C ATOM 1028 C THR A 73156.375 2.353 10.085 1.00 0.00 C ATOM 1029 O THR A 73155.407 2.245 10.838 1.00 0.00 O ATOM 1030 CB THR A 73157.569 4.194 11.287 1.00 0.00 C ATOM 1031 OG1 THR A 73157.769 5.596 11.260 1.00 0.00 O ATOM 1032 CG2 THR A 73158.861 3.554 11.744 1.00 0.00 C ATOM 1033 H THR A 73155.443 5.008 9.787 1.00 0.00 H ATOM 1034 HA THR A 73157.950 3.549 9.283 1.00 0.00 H ATOM 1035 HB THR A 73156.810 3.974 12.025 1.00 0.00 H ATOM 1036 HG1 THR A 73158.374 5.820 10.549 1.00 0.00 H ATOM 1037 1HG2 THR A 73158.644 2.615 12.232 1.00 0.00 H ATOM 1038 2HG2 THR A 73159.362 4.213 12.438 1.00 0.00 H ATOM 1039 3HG2 THR A 73159.498 3.378 10.890 1.00 0.00 H ATOM 1040 N CYS A 74156.856 1.339 9.374 1.00 0.00 N ATOM 1041 CA CYS A 74156.259 0.010 9.438 1.00 0.00 C ATOM 1042 C CYS A 74157.337 -1.069 9.474 1.00 0.00 C ATOM 1043 O CYS A 74158.530 -0.770 9.420 1.00 0.00 O ATOM 1044 CB CYS A 74155.333 -0.215 8.241 1.00 0.00 C ATOM 1045 SG CYS A 74153.621 0.290 8.527 1.00 0.00 S ATOM 1046 H CYS A 74157.629 1.488 8.790 1.00 0.00 H ATOM 1047 HA CYS A 74155.679 -0.049 10.346 1.00 0.00 H ATOM 1048 1HB CYS A 74155.705 0.347 7.398 1.00 0.00 H ATOM 1049 2HB CYS A 74155.329 -1.267 7.992 1.00 0.00 H ATOM 1050 HG CYS A 74153.631 1.051 9.113 1.00 0.00 H ATOM 1051 N ALAA 75156.908 -2.324 9.562 1.00 0.00 N ATOM 1052 CA ALAA 75157.836 -3.447 9.604 1.00 0.00 C ATOM 1053 C ALA A 75158.524 -3.641 8.257 1.00 0.00 C ATOM 1054 O ALAA 75158.192 -2.974 7.277 1.00 0.00 O

ATOM 1055 CB ALAA 75157.108 -4.718 10.014 1.00 0.00 C ATOM 1056 H ALAA 75155.945 -2.498 9.601 1.00 0.00 H ATOM 1057 HA ALAA 75158.586 -3.232 10.352 1.00 0.00 H ATOM 1058 1HB ALA A 75156.868 -5.295 9.134 1.00 0.00 H ATOM 1059 2HB ALA A 75156.197 -4.459 10.535 1.00 0.00 H ATOM 1060 3HB ALA A 75157.741 -5.301 10.666 1.00 0.00 H ATOM 1061 N LEUA 76159.485 -4.558 8.216 1.00 0.00 N ATOM 1062 CA LEU A 76160.222 -4.840 6.989 1.00 0.00 C ATOM 1063 C LEUA 76159.471 -5.846 6.123 1.00 0.00 C ATOM 1064 O LEUA 76158.917 -6.822 6.628 1.00 0.00 O ATOM 1065 CB LEU A 76161.617 -5.374 7.317 1.00 0.00 C ATOM 1066 CG LEUA 76162.644 -4.307 7.700 1.00 0.00 C ATOM 1067 CD1 LEU A 76163.639 -4.860 8.709 1.00 0.00 C ATOM 1068 CD2 LEU A 76163.367 -3.795 6.463 1.00 0.00 C ATOM 1069 H LEU A 76159.706 -5.056 9.031 1.00 0.00 H ATOM 1070 HA LEUA 76160.320 -3.914 6.442 1.00 0.00 H ATOM 1071 1HB LEU A 76161.529 -6.070 8.139 1.00 0.00 H ATOM 1072 2HB LEU A 76161.988 -5.905 6.455 1.00 0.00 H ATOM 1073 HG LEU A 76162.134 -3.472 8.159 1.00 0.00 H ATOM 1074 1HD1 LEU A 76163.261 -4.706 9.709 1.00 0.00 H ATOM 1075 2HD1 LEU A 76164.585 -4.352 8.600 1.00 0.00 H ATOM 1076 3HD1 LEU A 76163.777 -5.919 8.536 1.00 0.00 H ATOM 1077 1HD2 LEU A 76162.751 -3.963 5.592 1.00 0.00 H ATOM 1078 2HD2 LEU A 76164.302 -4.323 6.349 1.00 0.00 H ATOM 1079 3HD2 LEU A 76163.560 -2.739 6.570 1.00 0.00 H ATOM 1080 N LYS A 77159.456 -5.600 4.817 1.00 0.00 N ATOM 1081 CA LYS A 77158.773 -6.486 3.881 1.00 0.00 C ATOM 1082 C LYS A 77157.282 -6.563 4.193 1.00 0.00 C ATOM 1083 O LYS A 77156.676 -7.632 4.119 1.00 0.00 O ATOM 1084 CB LYS A 77159.390 -7.885 3.928 1.00 0.00 C ATOM 1085 CG LYS A 77160.875 -7.906 3.603 1.00 0.00 C

ATOM 1086 CD LYS A 77161.118 -7.884 2.103 1.00 0.00 C ATOM 1087 CE LYS A 77162.543 -7.467 1.776 1.00 0.00 C ATOM 1088 NZ LYS A 77163.090 -8.220 0.614 1.00 0.00 N ATOM 1089 H LYS A 77159.916 -4.805 4.475 1.00 0.00 H ATOM 1090 HA LYS A 77158.900 -6.079 2.889 1.00 0.00 H ATOM 1091 1HB LYS A 77159.255 -8.293 4.918 1.00 0.00 H ATOM 1092 2HB LYS A 77158.879 -8.515 3.215 1.00 0.00 H ATOM 1093 1HG LYS A 77161.343 -7.040 4.047 1.00 0.00 H ATOM 1094 2HG LYS A 77161.311 -8.804 4.017 1.00 0.00 H ATOM 1095 1HD LYS A 77160.944 -8.872 1.705 1.00 0.00 H ATOM 1096 2HD LYS A 77160.434 -7.183 1.648 1.00 0.00 H ATOM 1097 1HE LYS A 77162.551 -6.412 1.544 1.00 0.00 H ATOM 1098 2HE LYS A 77163.166 -7.649 2.639 1.00 0.00 H ATOM 1099 1HZ LYS A 77162.550 -7.995 -0.246 1.00 0.00 H ATOM 1100 2HZ LYS A 77163.028 -9.244 0.790 1.00 0.00 H ATOM 1101 3HZ LYS A 77164.088 -7.967 0.461 1.00 0.00 H ATOM 1102 N LYS A 78156.696 -5.423 4.544 1.00 0.00 N ATOM 1103 CA LYS A 78155.275 -5.362 4.868 1.00 0.00 C ATOM 1104 C LYS A 78154.692 -4.001 4.500 1.00 0.00 C ATOM 1105 O LYS A 78153.843 -3.465 5.212 1.00 0.00 O ATOM 1106 CB LYS A 78155.058 -5.638 6.357 1.00 0.00 C ATOM 1107 CG LYS A 78155.577 -6.994 6.806 1.00 0.00 C ATOM 1108 CD LYS A 78155.301 -7.234 8.282 1.00 0.00 C ATOM 1109 CE LYS A 78154.066 -8.098 8.483 1.00 0.00 C ATOM 1110 NZ LYS A 78153.349 -7.755 9.743 1.00 0.00 N ATOM 1111 H LYS A 78157.232 -4.604 4.586 1.00 0.00 H ATOM 1112 HA LYS A 78154.772 -6.123 4.293 1.00 0.00 H ATOM 1113 1HB LYS A 78155.565 -4.875 6.930 1.00 0.00 H ATOM 1114 2HB LYS A 78154.001 -5.592 6.569 1.00 0.00 H ATOM 1115 1HG LYS A 78155.089 -7.764 6.228 1.00 0.00 H ATOM 1116 2HG LYS A 78156.643 -7.035 6.636 1.00 0.00 H ATOM 1117 1HD LYS A 78156.152 -7.734 8.720 1.00 0.00 H ATOM 1118 2HD LYS A 78155.148 -6.283 8.769 1.00 0.00 H ATOM 1119 1HE LYS A 78153.399 -7.950 7.649 1.00 0.00 H ATOM 1120 2HE LYS A 78154.369 -9.134 8.522 1.00 0.00 H ATOM 1121 1HZ LYS A 78152.922 -8.610 10.155 1.00 0.00 H ATOM 1122 2HZ LYS A 78152.597 -7.065 9.549 1.00 0.00 H ATOM 1123 3HZ LYS A 78154.012 -7.345 10.431 1.00 0.00 H ATOM 1124 N ALA A 79155.152 -3.448 3.382 1.00 0.00 N ATOM 1125 CA ALA A 79154.674 -2.151 2.920 1.00 0.00 C ATOM 1126 C ALA A 79154.599 -2.103 1.397 1.00 0.00 C ATOM 1127 O ALA A 79155.621 -2.002 0.719 1.00 0.00 O ATOM 1128 CB ALA A 79155.576 -1.041 3.440 1.00 0.00 C ATOM 1129 H ALAA 79155.828 -3.923 2.856 1.00 0.00 H ATOM 1130 HA ALA A 79153.684 -1.996 3.324 1.00 0.00 H ATOM 1131 1HB ALAA 79155.178 -0.659 4.369 1.00 0.00 H ATOM 1132 2HB ALA A 79155.621 -0.243 2.714 1.00 0.00 H ATOM 1133 3HB ALA A 79156.569 -1.432 3.607 1.00 0.00 H ATOM 1134 N LEUA 80153.382 -2.177 0.868 1.00 0.00 N ATOM 1135 CA LEU A 80153.172 -2.143 -0.576 1.00 0.00 C ATOM 1136 C LEU A 80152.306 -0.951 -0.970 1.00 0.00 C ATOM 1137 O LEUA 80151.157 -0.836 -0.541 1.00 0.00 O ATOM 1138 CB LEU A 80152.518 -3.443 -1.047 1.00 0.00 C ATOM 1139 CG LEU A 80152.189 -3.497 -2.540 1.00 0.00 C ATOM 1140 CD1 LEU A 80153.449 -3.741 -3.356 1.00 0.00 C ATOM 1141 CD2 LEU A 80151.155 -4.579 -2.817 1.00 0.00 C ATOM 1142 H LEU A 80152.606 -2.257 1.462 1.00 0.00 H ATOM 1143 HA LEU A 80154.137 -2.043 -1.049 1.00 0.00 H ATOM 1144 1HB LEU A 80153.185 -4.261 -0.816 1.00 0.00 H ATOM 1145 2HB LEU A 80151.601 -3.581 -0.494 1.00 0.00 H ATOM 1146 HG LEU A 80151.772 -2.549 -2.845 1.00 0.00 H ATOM 1147 1HD1 LEU A 80153.391 -3.188 -4.282 1.00 0.00 H ATOM 1148 2HD1 LEU A 80153.541 -4.794 -3.571 1.00 0.00 H ATOM 1149 3HD1 LEU A 80154.311 -3.411 -2.794 1.00 0.00 H ATOM 1150 1HD2 LEU A 80150.553 -4.292 -3.666 1.00 0.00 H ATOM 1151 2HD2 LEU A 80150.522 -4.703 -1.951 1.00 0.00 H ATOM 1152 3HD2 LEU A 80151.658 -5.511 -3.032 1.00 0.00 H ATOM 1153 N PHE A 81152.863 -0.066 -1.789 1.00 0.00 N ATOM 1154 CA PHE A 81152.142 1.118 -2.242 1.00 0.00 C ATOM 1155 C PHE A 81151.299 0.803 -3.473 1.00 0.00 C ATOM 1156 O PHE A 81151.736 0.083 -4.371 1.00 0.00 O ATOM 1157 CB PHE A 81153.123 2.249 -2.557 1.00 0.00 C ATOM 1158 CG PHE A 81153.763 2.847 -1.336 1.00 0.00 C ATOM 1159 CD1 PHE A 81153.243 3.993 -0.757 1.00 0.00 C ATOM 1160 CD2 PHE A 81154.883 2.260 -0.768 1.00 0.00 C ATOM 1161 CE1 PHE A 81153.829 4.545 0.367 1.00 0.00 C ATOM 1162 CE2 PHE A 81155.473 2.808 0.355 1.00 0.00 C ATOM 1163 CZ PHE A 81154.946 3.952 0.923 1.00 0.00 C ATOM 1164 H PHE A 81153.783 -0.212 -2.096 1.00 0.00 H ATOM 1165 HA PHE A 81151.487 1.433 -1.443 1.00 0.00 H ATOM 1166 1HB PHE A 81153.910 1.868 -3.191 1.00 0.00 H ATOM 1167 2HB PHE A 81152.597 3.037 -3.077 1.00 0.00 H ATOM 1168 HD1 PHE A 81152.370 4.457 -1.190 1.00 0.00 H ATOM 1169 HD2 PHE A 81155.296 1.367 -1.212 1.00 0.00 H ATOM 1170 HE1 PHE A 81153.416 5.439 0.809 1.00 0.00 H ATOM 1171 HE2 PHE A 81156.346 2.343 0.788 1.00 0.00 H ATOM 1172 HZ PHE A 81155.407 4.381 1.802 1.00 0.00 H ATOM 1173 N VALA 82150.087 1.347 -3.509 1.00 0.00 N ATOM 1174 CA VALA 82149.182 1.124 -4.631 1.00 0.00 C ATOM 1175 C VALA 82148.297 2.342 -4.873 1.00 0.00 C ATOM 1176 O VALA 82148.200 3.229 -4.027 1.00 0.00 O ATOM 1177 CB VALA 82148.288 -0.107 -4.394 1.00 0.00 C ATOM 1178 CG1 VAL A 82149.115 -1.382 -4.425 1.00 0.00 C

ATOM 1179 CG2 VAL A 82147.539 0.021 -3.077 1.00 0.00 C ATOM 1180 H VALA 82149.794 1.912 -2.764 1.00 0.00 H ATOM 1181 HA VALA 82149.780 0.945 -5.512 1.00 0.00 H ATOM 1182 HB VALA 82147.561 -0.158 -5.192 1.00 0.00 H ATOM 1183 1HG1 VAL A 82149.562 -1.499 -5.401 1.00 0.00 H ATOM 1184 2HG1 VAL A 82148.478 -2.230 -4.217 1.00 0.00 H ATOM 1185 3HG1 VAL A 82149.893 -1.325 -3.677 1.00 0.00 H ATOM 1186 1HG2 VAL A 82147.408 -0.959 -2.641 1.00 0.00 H ATOM 1187 2HG2 VAL A 82146.572 0.469 -3.254 1.00 0.00 H ATOM 1188 3HG2 VAL A 82148.106 0.644 -2.400 1.00 0.00 H ATOM 1189 N LYS A 83147.652 2.375 -6.035 1.00 0.00 N ATOM 1190 CA LYS A 83146.774 3.484 -6.390 1.00 0.00 C ATOM 1191 C LYS A 83145.517 3.482 -5.528 1.00 0.00 C ATOM 1192 O LYS A 83144.750 2.518 -5.530 1.00 0.00 O ATOM 1193 CB LYS A 83146.392 3.406 -7.870 1.00 0.00 C ATOM 1194 CG LYS A 83147.588 3.405 -8.808 1.00 0.00 C ATOM 1195 CD LYS A 83147.168 3.152 -10.247 1.00 0.00 C ATOM 1196 CE LYS A 83147.976 3.993 -11.220 1.00 0.00 C ATOM 1197 NZ LYS A 83148.286 3.250 -12.472 1.00 0.00 N ATOM 1198 H LYS A 83147.770 1.637 -6.669 1.00 0.00 H ATOM 1199 HA LYS A 83147.313 4.403 -6.216 1.00 0.00 H ATOM 1200 1HB LYS A 83145.830 2.498 -8.038 1.00 0.00 H ATOM 1201 2HB LYS A 83145.770 4.254 -8.115 1.00 0.00 H ATOM 1202 1HG LYS A 83148.078 4.366 -8.751 1.00 0.00 H ATOM 1203 2HG LYS A 83148.274 2.630 -8.501 1.00 0.00 H ATOM 1204 1HD LYS A 83147.318 2.108 -10.477 1.00 0.00 H ATOM 1205 2HD LYS A 83146.121 3.398 -10.354 1.00 0.00 H ATOM 1206 1HE LYS A 83147.410 4.879 -11.469 1.00 0.00 H ATOM 1207 2HE LYS A 83148.902 4.282 -10.744 1.00 0.00 H ATOM 1208 1HZ LYS A 83149.234 3.508 -12.816 1.00 0.00 H ATOM 1209 2HZ LYS A 83147.589 3.481 -13.207 1.00 0.00 H

ATOM 1210 3HZ LYS A 83148.261 2.226 -12.296 1.00 0.00 H ATOM 1211 N LEUA 84145.313 4.569 -4.792 1.00 0.00 N ATOM 1212 CA LEU A 84144.151 4.700 -3.922 1.00 0.00 C ATOM 1213 C LEU A 84142.856 4.573 -4.719 1.00 0.00 C ATOM 1214 O LEUA 84141.863 4.038 -4.227 1.00 0.00 O ATOM 1215 CB LEU A 84144.189 6.045 -3.194 1.00 0.00 C ATOM 1216 CG LEU A 84142,978 6,339 -2,308 1.00 0.00 C ATOM 1217 CD1 LEU A 84143.141 5.682 -0.946 1.00 0.00 C ATOM 1218 CD2 LEU A 84142.780 7.840 -2.158 1.00 0.00 C ATOM 1219 H LEU A 84145.962 5.301 -4.836 1.00 0.00 H ATOM 1220 HA LEUA 84144.191 3.905 -3.193 1.00 0.00 H ATOM 1221 1HB LEU A 84145.075 6.071 -2.577 1.00 0.00 H ATOM 1222 2HB LEU A 84144.264 6.827 -3.934 1.00 0.00 H ATOM 1223 HG LEU A 84142.091 5.928 -2.771 1.00 0.00 H ATOM 1224 1HD1 LEU A 84143.630 4.727 -1.063 1.00 0.00 H ATOM 1225 2HD1 LEU A 84142.169 5.537 -0.497 1.00 0.00 H ATOM 1226 3HD1 LEU A 84143.739 6.318 -0.309 1.00 0.00 H ATOM 1227 1HD2 LEU A 84141.894 8.030 -1.571 1.00 0.00 H ATOM 1228 2HD2 LEU A 84142.667 8.287 -3.134 1.00 0.00 H ATOM 1229 3HD2 LEU A 84143.639 8.268 -1.663 1.00 0.00 H ATOM 1230 N LYS A 85142.875 5.070 -5.951 1.00 0.00 N ATOM 1231 CA LYS A 85141.701 5.014 -6.815 1.00 0.00 C ATOM 1232 C LYS A 85141.332 3.569 -7.138 1.00 0.00 C ATOM 1233 O LYS A 85140.173 3.263 -7.421 1.00 0.00 O ATOM 1234 CB LYS A 85141.958 5.788 -8.109 1.00 0.00 C ATOM 1235 CG LYS A 85143.098 5.223 -8.941 1.00 0.00 C ATOM 1236 CD LYS A 85143.604 6.236 -9.955 1.00 0.00 C ATOM 1237 CE LYS A 85144.941 5.817 -10.542 1.00 0.00 C ATOM 1238 NZ LYS A 85145.553 6.900 -11.362 1.00 0.00 N ATOM 1239 H LYS A 85143.696 5.486 -6.287 1.00 0.00 H ATOM 1240 HA LYS A 85140.879 5.473 -6.289 1.00 0.00 H

ATOM 1241 1HB LYS A 85141.060 5.770 -8.710 1.00 0.00 H ATOM 1242 2HB LYS A 85142.195 6.812 -7.862 1.00 0.00 H ATOM 1243 1HG LYS A 85143.910 4.952 -8.283 1.00 0.00 H ATOM 1244 2HG LYS A 85142.748 4.346 -9.465 1.00 0.00 H ATOM 1245 1HD LYS A 85142.882 6.323 -10.753 1.00 0.00 H ATOM 1246 2HD LYS A 85143.719 7.193 -9.466 1.00 0.00 H ATOM 1247 1HE LYS A 85145.613 5.567 -9.734 1.00 0.00 H ATOM 1248 2HE LYS A 85144.790 4.948 -11.165 1.00 0.00 H ATOM 1249 1HZ LYS A 85145.891 7.666 -10.746 1.00 0.00 H ATOM 1250 2HZ LYS A 85144.850 7.287 -12.023 1.00 0.00 H ATOM 1251 3HZ LYS A 85146.356 6.526 -11.906 1.00 0.00 H ATOM 1252 N SER A 86142.322 2.682 -7.094 1.00 0.00 N ATOM 1253 CA SER A 86142.098 1.271 -7.381 1.00 0.00 C ATOM 1254 C SER A 86142.057 0.453 -6.095 1.00 0.00 C ATOM 1255 O SER A 86142.443 -0.716 -6.079 1.00 0.00 O ATOM 1256 CB SER A 86143.194 0.737 -8.305 1.00 0.00 C ATOM 1257 OG SER A 86143.269 1.496 -9.499 1.00 0.00 O ATOM 1258 H SER A 86143.225 2.984 -6.862 1.00 0.00 H ATOM 1259 HA SER A 86141.144 1.182 -7.881 1.00 0.00 H ATOM 1260 1HB SER A 86144.146 0.792 -7.799 1.00 0.00 H ATOM 1261 2HB SER A 86142.980 -0.290 -8.558 1.00 0.00 H ATOM 1262 HG SER A 86142.385 1.639 -9.845 1.00 0.00 H ATOM 1263 N CYS A 87141.587 1.075 -5.018 1.00 0.00 N ATOM 1264 CA CYS A 87141.496 0.404 -3.726 1.00 0.00 C ATOM 1265 C CYS A 87140.043 0.114 -3.366 1.00 0.00 C ATOM 1266 O CYS A 87139.125 0.737 -3.901 1.00 0.00 O ATOM 1267 CB CYS A 87142.143 1.260 -2.637 1.00 0.00 C ATOM 1268 SG CYS A 87143.948 1.167 -2.600 1.00 0.00 S ATOM 1269 H CYS A 87141.296 2.007 -5.094 1.00 0.00 H ATOM 1270 HA CYS A 87142.029 -0.532 -3.801 1.00 0.00 H ATOM 1271 1HB CYS A 87141.871 2.293 -2.792 1.00 0.00 H

ATOM 1272 2HB CYS A 87141.777 0.938 -1.673 1.00 0.00 H ATOM 1273 HG CYS A 87144.265 1.809 -1.959 1.00 0.00 H ATOM 1274 N ARG A 88139.840 -0.834 -2.458 1.00 0.00 N ATOM 1275 CA ARG A 88138.497 -1.205 -2.028 1.00 0.00 C ATOM 1276 C ARG A 88138.413 -1.271 -0.503 1.00 0.00 C ATOM 1277 O ARG A 88139.296 -1.826 0.151 1.00 0.00 O ATOM 1278 CB ARG A 88138.102 -2.555 -2.631 1.00 0.00 C ATOM 1279 CG ARG A 88137.308 -2.435 -3.921 1.00 0.00 C ATOM 1280 CD ARG A 88135.810 -2.459 -3.658 1.00 0.00 C ATOM 1281 NE ARG A 88135.049 -1.912 -4.778 1.00 0.00 N ATOM 1282 CZ ARG A 88133.789 -1.490 -4.682 1.00 0.00 C ATOM 1283 NH1 ARG A 88133.148 -1.550 -3.522 1.00 0.00 N ATOM 1284 NH2 ARG A 88133.171 -1.005 -5.749 1.00 0.00 N ATOM 1285 H ARG A 88140.612 -1.296 -2.068 1.00 0.00 H ATOM 1286 HA ARGA 88137.816 -0.449 -2.386 1.00 0.00 H ATOM 1287 1HB ARG A 88138.998 -3.121 -2.836 1.00 0.00 H ATOM 1288 2HB ARG A 88137.502 -3.096 -1.914 1.00 0.00 H ATOM 1289 1HG ARG A 88137.563 -1.504 -4.405 1.00 0.00 H ATOM 1290 2HG ARG A 88137.564 -3.262 -4.568 1.00 0.00 H ATOM 1291 1HD ARG A 88135.504 -3.481 -3.491 1.00 0.00 H ATOM 1292 2HD ARG A 88135.604 -1.873 -2.773 1.00 0.00 H ATOM 1293 HE ARGA 88135.498 -1.856 -5.647 1.00 0.00 H ATOM 1294 1HH1 ARG A 88133.608 -1.915 -2.713 1.00 0.00 H ATOM 1295 2HH1 ARG A 88132.203 -1.231 -3.456 1.00 0.00 H ATOM 1296 1HH2 ARG A 88133.649 -0.958 -6.626 1.00 0.00 H ATOM 1297 2HH2 ARG A 88132.225 -0.688 -5.678 1.00 0.00 H ATOM 1298 N PRO A 89137.344 -0.704 0.089 1.00 0.00 N ATOM 1299 CA PRO A 89137.157 -0.707 1.544 1.00 0.00 C ATOM 1300 C PRO A 89137.223 -2.113 2.132 1.00 0.00 C ATOM 1301 O PRO A 89136.564 -3.031 1.646 1.00 0.00 O ATOM 1302 CB PRO A 89135.757 -0.117 1.729 1.00 0.00 C

ATOM 1303 CG PRO A 89135.519 0.693 0.503 1.00 0.00 C ATOM 1304 CD PRO A 89136.239 -0.019 -0.608 1.00 0.00 C ATOM 1305 HA PRO A 89137.884 -0.079 2.037 1.00 0.00 H ATOM 1306 1HB PRO A 89135.037 -0.916 1.822 1.00 0.00 H ATOM 1307 2HB PRO A 89135.737 0.498 2.617 1.00 0.00 H ATOM 1308 1HG PRO A 89134.461 0.740 0.294 1.00 0.00 H ATOM 1309 2HG PRO A 89135.922 1.686 0.635 1.00 0.00 H ATOM 1310 1HD PRO A 89135.584 -0.732 -1.086 1.00 0.00 H ATOM 1311 2HD PRO A 89136.619 0.691 -1.326 1.00 0.00 H ATOM 1312 N ASP A 90138.021 -2.273 3.183 1.00 0.00 N ATOM 1313 CA ASP A 90138.172 -3.568 3.838 1.00 0.00 C ATOM 1314 C ASPA 90137.378 -3.612 5.140 1.00 0.00 C ATOM 1315 O ASPA 90137.759 -2.992 6.133 1.00 0.00 O ATOM 1316 CB ASP A 90139.648 -3.854 4.116 1.00 0.00 C ATOM 1317 CG ASP A 90139.948 -5.339 4.174 1.00 0.00 C ATOM 1318 OD1 ASP A 90140.366 -5.819 5.248 1.00 0.00 O ATOM 1319 OD2 ASP A 90139.764 -6.022 3.144 1.00 0.00 O ATOM 1320 H ASP A 90138.520 -1.503 3.526 1.00 0.00 H ATOM 1321 HA ASPA 90137.787 -4.323 3.170 1.00 0.00 H ATOM 1322 1HB ASPA 90140.247 -3.414 3.333 1.00 0.00 H ATOM 1323 2HB ASPA 90139.921 -3.412 5.063 1.00 0.00 H ATOM 1324 N SER A 91136.274 -4.352 5.129 1.00 0.00 N ATOM 1325 CA SER A 91135.426 -4.478 6.310 1.00 0.00 C ATOM 1326 C SER A 91135.724 -5.774 7.057 1.00 0.00 C ATOM 1327 O SER A 91134.840 -6.355 7.688 1.00 0.00 O ATOM 1328 CB SER A 91133.950 -4.434 5.911 1.00 0.00 C ATOM 1329 OG SER A 91133.158 -3.879 6.947 1.00 0.00 O ATOM 1330 H SER A 91136.023 -4.823 4.308 1.00 0.00 H ATOM 1331 HA SER A 91135.639 -3.644 6.961 1.00 0.00 H ATOM 1332 1HB SER A 91133.837 -3.827 5.024 1.00 0.00 H ATOM 1333 2HB SER A 91133.605 -5.436 5.708 1.00 0.00 H

ATOM 1334 HG SER A 91132.243 -3.834 6.660 1.00 0.00 H ATOM 1335 N ARG A 92136.972 -6.223 6.981 1.00 0.00 N ATOM 1336 CA ARG A 92137.384 -7.451 7.650 1.00 0.00 C ATOM 1337 C ARG A 92137.327 -7.291 9.166 1.00 0.00 C ATOM 1338 O ARG A 92137.085 -8.254 9.893 1.00 0.00 O ATOM 1339 CB ARG A 92138.798 -7.842 7.220 1.00 0.00 C ATOM 1340 CG ARG A 92138.835 -8.741 5.995 1.00 0.00 C ATOM 1341 CD ARG A 92140.147 -9.503 5.902 1.00 0.00 C ATOM 1342 NE ARG A 92140.288 -10.485 6.976 1.00 0.00 N ATOM 1343 CZ ARG A 92139.667 -11.663 6.989 1.00 0.00 C ATOM 1344 NH1 ARG A 92138.865 -12.010 5.991 1.00 0.00 N ATOM 1345 NH2 ARG A 92139.851 -12.496 8.004 1.00 0.00 N ATOM 1346 H ARG A 92137.632 -5.717 6.462 1.00 0.00 H ATOM 1347 HA ARG A 92136.700 -8.234 7.358 1.00 0.00 H ATOM 1348 1HB ARG A 92139.355 -6.944 6.997 1.00 0.00 H ATOM 1349 2HB ARG A 92139.281 -8.361 8.035 1.00 0.00 H ATOM 1350 1HG ARG A 92138.022 -9.450 6.056 1.00 0.00 H ATOM 1351 2HG ARG A 92138.719 -8.133 5.109 1.00 0.00 H ATOM 1352 1HD ARG A 92140.185 -10.016 4.953 1.00 0.00 H ATOM 1353 2HD ARG A 92140.963 -8.798 5.962 1.00 0.00 H ATOM 1354 HE ARG A 92140.875 -10.253 7.725 1.00 0.00 H ATOM 1355 1HH1 ARG A 92138.722 -11.386 5.223 1.00 0.00 H ATOM 1356 2HH1 ARG A 92138.403 -12.896 6.007 1.00 0.00 H ATOM 1357 1HH2 ARG A 92140.455 -12.240 8.758 1.00 0.00 H ATOM 1358 2HH2 ARG A 92139.385 -13.381 8.014 1.00 0.00 H ATOM 1359 N PHE A 93137.554 -6.068 9.637 1.00 0.00 N ATOM 1360 CA PHE A 93137.528 -5.782 11.067 1.00 0.00 C ATOM 1361 C PHE A 93136.525 -4.678 11.385 1.00 0.00 C ATOM 1362 O PHE A 93136.707 -3.917 12.335 1.00 0.00 O ATOM 1363 CB PHE A 93138.921 -5.377 11.551 1.00 0.00 C ATOM 1364 CG PHE A 93139.888 -6.524 11.626 1.00 0.00 C

ATOM 1365 CD1 PHE A 93140.464 -6.884 12.834 1.00 0.00 C ATOM 1366 CD2 PHE A 93140.221 -7.243 10.489 1.00 0.00 C ATOM 1367 CE1 PHE A 93141.354 -7.938 12.907 1.00 0.00 C ATOM 1368 CE2 PHE A 93141.111 -8.298 10.555 1.00 0.00 C ATOM 1369 CZ PHE A 93141.677 -8.646 11.765 1.00 0.00 C ATOM 1370 H PHE A 93137.741 -5.341 9.007 1.00 0.00 H ATOM 1371 HA PHE A 93137.227 -6.684 11.579 1.00 0.00 H ATOM 1372 1HB PHE A 93139.330 -4.642 10.874 1.00 0.00 H ATOM 1373 2HB PHE A 93138.839 -4.945 12.537 1.00 0.00 H ATOM 1374 HD1 PHE A 93140.212 -6.330 13.727 1.00 0.00 H ATOM 1375 HD2 PHE A 93139.778 -6.971 9.543 1.00 0.00 H ATOM 1376 HE1 PHE A 93141.796 -8.208 13.854 1.00 0.00 H ATOM 1377 HE2 PHE A 93141.361 -8.850 9.662 1.00 0.00 H ATOM 1378 HZ PHE A 93142.373 -9.471 11.820 1.00 0.00 H ATOM 1379 N ALAA 94135.467 -4.596 10.586 1.00 0.00 N ATOM 1380 CA ALA A 94134.436 -3.584 10.785 1.00 0.00 C ATOM 1381 C ALA A 94133.274 -4.138 11.602 1.00 0.00 C ATOM 1382 O ALAA 94132.658 -5.136 11.227 1.00 0.00 O ATOM 1383 CB ALA A 94133.940 -3.064 9.444 1.00 0.00 C ATOM 1384 H ALA A 94135.376 -5.231 9.844 1.00 0.00 H ATOM 1385 HA ALA A 94134.879 -2.759 11.322 1.00 0.00 H ATOM 1386 1HB ALA A 94133.035 -3.584 9.169 1.00 0.00 H ATOM 1387 2HB ALA A 94134.696 -3.235 8.691 1.00 0.00 H ATOM 1388 3HB ALA A 94133.739 -2.007 9.520 1.00 0.00 H ATOM 1389 N SER A 95132.980 -3.485 12.721 1.00 0.00 N ATOM 1390 CA SER A 95131.891 -3.913 13.593 1.00 0.00 C ATOM 1391 C SER A 95130.740 -2.913 13.557 1.00 0.00 C ATOM 1392 O SER A 95130.944 -1.724 13.314 1.00 0.00 O ATOM 1393 CB SER A 95132.394 -4.078 15.028 1.00 0.00 C ATOM 1394 OG SER A 95131.383 -4.612 15.865 1.00 0.00 O ATOM 1395 H SER A 95133.508 -2.696 12.967 1.00 0.00 H

ATOM 1396 HA SER A 95131.535 -4.867 13.234 1.00 0.00 H ATOM 1397 1HB SER A 95133.240 -4.748 15.035 1.00 0.00 H ATOM 1398 2HB SER A 95132.695 -3.115 15.415 1.00 0.00 H ATOM 1399 HG SER A 95131.061 -5.436 15.493 1.00 0.00 H ATOM 1400 N LEU A 96129.529 -3.404 13.802 1.00 0.00 N ATOM 1401 CA LEU A 96128.344 -2.554 13.798 1.00 0.00 C ATOM 1402 C LEUA 96127.403 -2.931 14.938 1.00 0.00 C ATOM 1403 O LEU A 96126.670 -3.916 14.852 1.00 0.00 O ATOM 1404 CB LEU A 96127.616 -2.665 12.456 1.00 0.00 C ATOM 1405 CG LEU A 96127.763 -1.451 11.537 1.00 0.00 C ATOM 1406 CD1 LEU A 96129.230 -1.182 11.239 1.00 0.00 C ATOM 1407 CD2 LEU A 96126.985 -1.664 10.247 1.00 0.00 C ATOM 1408 H LEUA 96129.430 -4.361 13.989 1.00 0.00 H ATOM 1409 HA LEUA 96128.669 -1.534 13.938 1.00 0.00 H ATOM 1410 1HB LEU A 96127.996 -3.533 11.936 1.00 0.00 H ATOM 1411 2HB LEU A 96126.564 -2.816 12.649 1.00 0.00 H ATOM 1412 HG LEU A 96127.358 -0.581 12.034 1.00 0.00 H ATOM 1413 1HD1 LEU A 96129.616 -0.468 11.952 1.00 0.00 H ATOM 1414 2HD1 LEU A 96129.327 -0.782 10.241 1.00 0.00 H ATOM 1415 3HD1 LEU A 96129.788 -2.103 11.315 1.00 0.00 H ATOM 1416 1HD2 LEU A 96125.972 -1.959 10.481 1.00 0.00 H ATOM 1417 2HD2 LEU A 96127.460 -2.438 9.663 1.00 0.00 H ATOM 1418 3HD2 LEU A 96126.969 -0.743 9.681 1.00 0.00 H ATOM 1419 N GLN A 97127.429 -2.139 16.006 1.00 0.00 N ATOM 1420 CA GLN A 97126.577 -2.389 17.163 1.00 0.00 C ATOM 1421 C GLN A 97126.881 -3.753 17.778 1.00 0.00 C ATOM 1422 O GLN A 97126.251 -4.753 17.433 1.00 0.00 O ATOM 1423 CB GLN A 97125.102 -2.314 16.763 1.00 0.00 C ATOM 1424 CG GLN A 97124.743 -1.048 16.001 1.00 0.00 C ATOM 1425 CD GLN A 97124.686 0.175 16.897 1.00 0.00 C ATOM 1426 OE1 GLN A 97123.756 0.338 17.686 1.00 0.00 O

ATOM 1427 NE2 GLN A 97125.684 1.041 16.778 1.00 0.00 N ATOM 1428 H GLN A 97128.035 -1.369 16.015 1.00 0.00 H ATOM 1429 HA GLN A 97126.782 -1.623 17.896 1.00 0.00 H ATOM 1430 1HB GLN A 97124.867 -3.162 16.139 1.00 0.00 H ATOM 1431 2HB GLN A 97124.497 -2.355 17.656 1.00 0.00 H ATOM 1432 1HG GLN A 97125.485 -0.880 15.236 1.00 0.00 H ATOM 1433 2HG GLN A 97123.775 -1.184 15.540 1.00 0.00 H ATOM 1434 1HE2 GLN A 97126.392 0.846 16.128 1.00 0.00 H ATOM 1435 2HE2 GLN A 97125.673 1.841 17.345 1.00 0.00 H ATOM 1436 N PRO A 98127.854 -3.812 18.702 1.00 0.00 N ATOM 1437 CA PRO A 98128.239 -5.063 19.366 1.00 0.00 C ATOM 1438 C PRO A 98127.043 -5.789 19.971 1.00 0.00 C ATOM 1439 O PRO A 98127.044 -7.014 20.094 1.00 0.00 O ATOM 1440 CB PRO A 98129.197 -4.602 20.467 1.00 0.00 C ATOM 1441 CG PRO A 98129.755 -3.315 19.969 1.00 0.00 C ATOM 1442 CD PRO A 98128.656 -2.668 19.173 1.00 0.00 C ATOM 1443 HA PRO A 98128.755 -5.726 18.689 1.00 0.00 H ATOM 1444 1HB PRO A 98128.652 -4.467 21.389 1.00 0.00 H ATOM 1445 2HB PRO A 98129.973 -5.341 20.605 1.00 0.00 H ATOM 1446 1HG PRO A 98130.034 -2.688 20.803 1.00 0.00 H ATOM 1447 2HG PRO A 98130.611 -3.505 19.338 1.00 0.00 H ATOM 1448 1HD PRO A 98128.067 -2.017 19.803 1.00 0.00 H ATOM 1449 2HD PRO A 98129.067 -2.117 18.340 1.00 0.00 H ATOM 1450 N SER A 99126.021 -5.025 20.346 1.00 0.00 N ATOM 1451 CA SER A 99124.818 -5.596 20.940 1.00 0.00 C ATOM 1452 C SER A 99123.564 -4.983 20.323 1.00 0.00 C ATOM 1453 O SER A 99123.584 -3.845 19.855 1.00 0.00 O ATOM 1454 CB SER A 99124.815 -5.377 22.453 1.00 0.00 C ATOM 1455 OG SER A 99125.417 -6.469 23.127 1.00 0.00 O ATOM 1456 H SER A 99126.079 -4.054 20.222 1.00 0.00 H ATOM 1457 HA SER A 99124.820 -6.657 20.738 1.00 0.00 H

ATOM 1458 1HB SER A 99125.367 -4.479 22.686 1.00 0.00 H ATOM 1459 2HB SER A 99123.797 -5.273 22.798 1.00 0.00 H ATOM 1460 HG SER A 99124.734 -7.021 23.516 1.00 0.00 H ATOM 1461 N GLY A 100122.475 -5.744 20.327 1.00 0.00 N ATOM 1462 CA GLY A 100121.229 -5.258 19.766 1.00 0.00 C ATOM 1463 C GLY A 100120.594 -4.171 20.614 1.00 0.00 C ATOM 1464 O GLY A 100120.434 -3.039 20.157 1.00 0.00 O ATOM 1465 H GLY A 100122.518 -6.644 20.714 1.00 0.00 H ATOM 1466 1HA GLY A 100121.420 -4.864 18.779 1.00 0.00 H ATOM 1467 2HA GLY A 100120.537 -6.085 19.685 1.00 0.00 H ATOM 1468 N PRO A 101120.221 -4.486 21.866 1.00 0.00 N ATOM 1469 CA PRO A 101119.600 -3.515 22.773 1.00 0.00 C ATOM 1470 C PRO A 101120.582 -2.443 23.233 1.00 0.00 C ATOM 1471 O PRO A 101121.475 -2.709 24.038 1.00 0.00 O ATOM 1472 CB PRO A 101119.150 -4.372 23.959 1.00 0.00 C ATOM 1473 CG PRO A 101120.062 -5.549 23.942 1.00 0.00 C ATOM 1474 CD PRO A 101120.374 -5.812 22.495 1.00 0.00 C ATOM 1475 HA PRO A 101118.741 -3.043 22.319 1.00 0.00 H ATOM 1476 1HB PRO A 101119.249 -3.806 24.873 1.00 0.00 H ATOM 1477 2HB PRO A 101118.121 -4.669 23.821 1.00 0.00 H ATOM 1478 1HG PRO A 101120.966 -5.320 24.485 1.00 0.00 H ATOM 1479 2HG PRO A 101119.566 -6.403 24.379 1.00 0.00 H ATOM 1480 1HD PRO A 101121.386 -6.175 22.387 1.00 0.00 H ATOM 1481 2HD PRO A 101119.671 -6.518 22.079 1.00 0.00 H ATOM 1482 N SER A 102120.410 -1.230 22.718 1.00 0.00 N ATOM 1483 CA SER A 102121.282 -0.117 23.077 1.00 0.00 C ATOM 1484 C SER A 102120.786 0.576 24.341 1.00 0.00 C ATOM 1485 O SER A 102121.581 1.051 25.153 1.00 0.00 O ATOM 1486 CB SER A 102121.358 0.889 21.926 1.00 0.00 C ATOM 1487 OG SER A 102120.064 1.307 21.527 1.00 0.00 O ATOM 1488 H SER A 102119.679 -1.080 22.081 1.00 0.00 H

ATOM 1489 HA SER A 102122.268 -0.515 23.261 1.00 0.00 H ATOM 1490 1HB SER A 102121.918 1.755 22.245 1.00 0.00 H ATOM 1491 2HB SER A 102121.851 0.430 21.082 1.00 0.00 H ATOM 1492 HG SER A 102119.966 2.248 21.690 1.00 0.00 H ATOM 1493 N SER A 103119.468 0.630 24.503 1.00 0.00 N ATOM 1494 CA SER A 103118.867 1.265 25.670 1.00 0.00 C ATOM 1495 C SER A 103119.270 0.543 26.952 1.00 0.00 C ATOM 1496 O SER A 103118.782 -0.550 27.240 1.00 0.00 O ATOM 1497 CB SER A 103117.343 1.283 25.539 1.00 0.00 C ATOM 1498 OG SER A 103116.799 2.484 26.058 1.00 0.00 O ATOM 1499 H SER A 103118.886 0.234 23.821 1.00 0.00 H ATOM 1500 HA SER A 103119.226 2.282 25.716 1.00 0.00 H ATOM 1501 1HB SER A 103117.073 1.202 24.497 1.00 0.00 H ATOM 1502 2HB SER A 103116.927 0.448 26.083 1.00 0.00 H ATOM 1503 HG SER A 103116.312 2.293 26.864 1.00 0.00 H ATOM 1504 N GLY A 104120.165 1.160 27.717 1.00 0.00 N ATOM 1505 CA GLY A 104120.618 0.561 28.957 1.00 0.00 C ATOM 1506 C GLY A 104119.539 0.545 30.022 1.00 0.00 C ATOM 1507 O GLY A 104119.748 -0.103 31.070 1.00 0.00 O ATOM 1508 OXT GLY A 104118.485 1.179 29.809 1.00 0.00 O ATOM 1509 H GLY A 104120.520 2.029 27.436 1.00 0.00 H ATOM 1510 1HA GLY A 104120.930 -0.455 28.762 1.00 0.00 H ATOM 1511 2HA GLY A 104121.464 1.121 29.327 1.00 0.00 H TER 1512 GLY A 104 **ENDMDL**

Three-Dimensional Structure Coordinate Table 2

ATOM 1 N GLY A 1105.215 7.354 -0.195 1.00 0.00 N ATOM 2 CA GLY A 1106.288 6.361 -0.481 1.00 0.00 C ATOM 3 C GLY A 1107.290 6.250 0.651 1.00 0.00 C ATOM 4 O GLY A 1107.077 6.795 1.734 1.00 0.00 O ATOM 5 1H GLY A 1105.533 8.026 0.533 1.00 0.00 H ATOM 6 2H GLY A 1104.360 6.869 0.147 1.00 0.00 H ATOM 7 3H GLY A 1104.976 7.882 -1.060 1.00 0.00 H ATOM 8 1HA GLY A 1105.834 5.395 -0.642 1.00 0.00 H ATOM 9 2HA GLY A 1106.807 6.659 -1.380 1.00 0.00 H ATOM10 N SER A 2108.386 5.542 0.400 1.00 0.00 N ATOM11 CA SER A 2109.426 5.360 1.405 1.00 0.00 C ATOM12 C SER A 2110.256 6.629 1.565 1.00 0.00 C ATOM13 O SER A 2110.259 7.496 0.691 1.00 0.00 O ATOM14 CB SER A 2110.332 4.187 1.026 1.00 0.00 C ATOM15 OG SER A 2109.867 2.977 1.597 1.00 0.00 O ATOM16 H SER A 2108.498 5.132 -0.484 1.00 0.00 H ATOM17 HA SER A 2108.942 5.140 2.346 1.00 0.00 H ATOM18 1HB SER A 2110.348 4.080 -0.048 1.00 0.00 H ATOM19 2HB SER A 2111.334 4.379 1.384 1.00 0.00 H ATOM20 HG SER A 2110.095 2.955 2.530 1.00 0.00 H ATOM21 N SER A 3110.962 6.731 2.687 1.00 0.00 N ATOM22 CA SER A 3111.797 7.894 2.960 1.00 0.00 C ATOM23 C SER A 3113.078 7.853 2.131 1.00 0.00 C ATOM24 O SER A 3113.500 8.866 1.573 1.00 0.00 O ATOM25 CB SER A 3112.142 7.961 4.450 1.00 0.00 C ATOM26 OG SER A 3113.199 7.072 4.769 1.00 0.00 O ATOM27 H SER A 3110.920 6.008 3.346 1.00 0.00 H ATOM28 HA SER A 3111.237 8.777 2.690 1.00 0.00 H ATOM29 1HB SER A 3112.447 8.967 4.702 1.00 0.00 H ATOM30 2HB SER A 3111.272 7.692 5.031 1.00 0.00 H ATOM31 HG SER A 3112.849 6.184 4.872 1.00 0.00 H ATOM32 N GLYA 4113.690 6.676 2.056 1.00 0.00 N ATOM33 CA GLY A 4114.915 6.525 1.294 1.00 0.00 C ATOM34 C GLYA 4116.155 6.661 2.156 1.00 0.00 C ATOM35 O GLY A 4116.173 7.435 3.112 1.00 0.00 O

ATOM36 H GLY A 4113.307 5.904 2.523 1.00 0.00 H ATOM37 1HA GLY A 4114.918 5.550 0.828 1.00 0.00 H ATOM38 2HA GLY A 4114.941 7.280 0.523 1.00 0.00 H ATOM39 N SER A 5117.194 5.905 1.817 1.00 0.00 N ATOM40 CA SER A 5118.444 5.943 2.567 1.00 0.00 C ATOM41 C SER A 5119.548 5.197 1.823 1.00 0.00 C ATOM42 O SER A 5119.739 3.997 2.018 1.00 0.00 O ATOM43 CB SER A 5118.248 5.336 3.957 1.00 0.00 C ATOM44 OG SER A 5117.949 3.954 3.871 1.00 0.00 O ATOM45 H SER A 5117.119 5.306 1.044 1.00 0.00 H ATOM46 HA SER A 5118.734 6.978 2.673 1.00 0.00 H ATOM47 1HB SER A 5119.154 5.461 4.533 1.00 0.00 H ATOM48 2HB SER A 5117.433 5.839 4.455 1.00 0.00 H ATOM49 HG SER A 5117.186 3.826 3.304 1.00 0.00 H ATOM50 N SER A 6120.271 5.917 0.971 1.00 0.00 N ATOM51 CA SER A 6121.355 5.322 0.198 1.00 0.00 C ATOM52 C SER A 6122.687 5.469 0.929 1.00 0.00 C ATOM53 O SER A 6123.365 6.489 0.805 1.00 0.00 O ATOM54 CB SER A 6121.443 5.975 -1.182 1.00 0.00 C ATOM55 OG SER A 6120.178 5.990 -1.821 1.00 0.00 O ATOM56 H SER A 6120.070 6.869 0.859 1.00 0.00 H ATOM57 HA SER A 6121.140 4.271 0.077 1.00 0.00 H ATOM58 1HB SER A 6121.790 6.992 -1.076 1.00 0.00 H ATOM59 2HB SER A 6122.137 5.420 -1.796 1.00 0.00 H ATOM60 HG SER A 6119.653 6.716 -1.475 1.00 0.00 H ATOM61 N GLY A 7123.055 4.444 1.688 1.00 0.00 N ATOM62 CA GLY A 7124.304 4.477 2.428 1.00 0.00 C ATOM63 C GLY A 7125.284 3.418 1.960 1.00 0.00 C ATOM64 O GLY A 7126.040 2.867 2.760 1.00 0.00 O ATOM65 H GLY A 7122.474 3.656 1.750 1.00 0.00 H ATOM66 1HA GLY A 7124.757 5.450 2.304 1.00 0.00 H

ATOM67 2HA GLY A 7124.095 4.321 3.475 1.00 0.00 H ATOM68 N LEUA 8125.269 3.134 0.662 1.00 0.00 N ATOM69 CA LEU A 8126.163 2.134 0.089 1.00 0.00 C ATOM70 C LEUA 8127.308 2.798 -0.668 1.00 0.00 C ATOM71 O LEUA 8128.424 2.279 -0.705 1.00 0.00 O ATOM72 CB LEU A 8125.389 1.205 -0.847 1.00 0.00 C ATOM73 CG LEU A 8124.503 0.173 -0.148 1.00 0.00 C ATOM74 CD1 LEU A 8123.307 -0.182 -1.018 1.00 0.00 C ATOM75 CD2 LEU A 8125.306 -1.075 0.192 1.00 0.00 C ATOM76 H LEUA 8124.644 3.608 0.076 1.00 0.00 H ATOM77 HA LEU A 8126.573 1.553 0.901 1.00 0.00 H ATOM78 1HB LEU A 8124.763 1.811 -1.486 1.00 0.00 H ATOM79 2HB LEU A 8126.099 0.676 -1.465 1.00 0.00 H ATOM80 HG LEU A 8124.130 0.594 0.775 1.00 0.00 H ATOM81 1HD1 LEU A 8122.467 -0.437 -0.390 1.00 0.00 H ATOM82 2HD1 LEU A 8123.557 -1.026 -1.646 1.00 0.00 H ATOM83 3HD1 LEU A 8123.050 0.664 -1.638 1.00 0.00 H ATOM84 1HD2 LEU A 8124.669 -1.943 0.118 1.00 0.00 H ATOM85 2HD2 LEU A 8125.689 -0.992 1.198 1.00 0.00 H ATOM86 3HD2 LEU A 8126.129 -1.171 -0.500 1.00 0.00 H ATOM87 N ALAA 9127.025 3.949 -1.271 1.00 0.00 N ATOM88 CA ALA A 9128.032 4.684 -2.027 1.00 0.00 C ATOM89 C ALAA 9128.353 6.018 -1.362 1.00 0.00 C ATOM90 O ALAA 9127.467 6.685 -0.828 1.00 0.00 O ATOM91 CB ALA A 9127.559 4.904 -3.456 1.00 0.00 C ATOM92 H ALAA 9126.117 4.312 -1.204 1.00 0.00 H ATOM93 HA ALA A 9128.930 4.083 -2.058 1.00 0.00 H ATOM94 1HB ALA A 9126.948 4.070 -3.766 1.00 0.00 H ATOM95 2HB ALA A 9128.415 4.986 -4.110 1.00 0.00 H ATOM96 3HB ALA A 9126.979 5.813 -3.507 1.00 0.00 H ATOM97 N META 10129.625 6.399 -1.399 1.00 0.00 N

ATOM98 CA META 10130.064 7.654 -0.799 1.00 0.00 C ATOM99 C META 10131.140 8.320 -1.656 1.00 0.00 C 100 O MET A 10132.329 8.052 -1.490 1.00 0.00 O 101 CB MET A 10130.601 7.410 0.612 1.00 0.00 C ATOM 102 CG MET A 10129.515 7.117 1.634 1.00 0.00 C **ATOM** 103 SD MET A 10130.052 5.956 2.905 1.00 0.00 S **ATOM** 104 CE MET A 10128.479 5.283 3.435 1.00 0.00 C **ATOM** 105 H MET A 10130.285 5.823 -1.839 1.00 0.00 H **ATOM** 106 HA META 10129.209 8.311 -0.740 1.00 0.00 H **ATOM** 107 1HB MET A 10131.277 6.568 0.586 1.00 0.00 H **ATOM** 108 2HB META 10131.144 8.286 0.935 1.00 0.00 H **ATOM** 109 1HG MET A 10129.229 8.043 2.110 1.00 0.00 H **ATOM** 110 2HG MET A 10128.661 6.699 1.121 1.00 0.00 H ATOM 111 1HE MET A 10127.696 6.001 3.239 1.00 0.00 H **ATOM ATOM** 112 2HE MET A 10128.516 5.071 4.493 1.00 0.00 H 113 3HE MET A 10128.277 4.371 2.892 1.00 0.00 H **ATOM** 114 N PRO A 11130.733 9.201 -2.588 1.00 0.00 N **ATOM** 115 CA PRO A 11131.672 9.903 -3.467 1.00 0.00 C ATOM **ATOM** 116 C PRO A 11132.708 10.710 -2.687 1.00 0.00 C 117 O PRO A 11133.901 10.639 -2.976 1.00 0.00 O **ATOM ATOM** 118 CB PRO A 11130.781 10.836 -4.295 1.00 0.00 C 119 CG PRO A 11129.406 10.270 -4.185 1.00 0.00 C **ATOM** 120 CD PRO A 11129.335 9.581 -2.851 1.00 0.00 C **ATOM** 121 HA PRO A 11132.181 9.214 -4.125 1.00 0.00 H ATOM 122 1HB PRO A 11130.831 11.836 -3.892 1.00 0.00 H ATOM 123 2HB PRO A 11131.120 10.841 -5.321 1.00 0.00 H ATOM 124 1HG PRO A 11128.680 11.066 -4.229 1.00 0.00 H **ATOM** 125 2HG PRO A 11129.236 9.561 -4.981 1.00 0.00 H ATOM 126 1HD PRO A 11128.971 10.260 -2.095 1.00 0.00 H ATOM 127 2HD PRO A 11128.704 8.707 -2.911 1.00 0.00 H ATOM 128 N PRO A 12132.269 11.487 -1.678 1.00 0.00 N ATOM

129 CA PRO A 12133.179 12.297 -0.861 1.00 0.00 C ATOM 130 C PRO A 12134.284 11.455 -0.232 1.00 0.00 C ATOM **ATOM** 131 O PRO A 12135.340 11.970 0.133 1.00 0.00 O ATOM 132 CB PRO A 12132.272 12.882 0.225 1.00 0.00 C 133 CG PRO A 12130.903 12.847 -0.360 1.00 0.00 C **ATOM** 134 CD PRO A 12130.866 11.636 -1.249 1.00 0.00 C **ATOM ATOM** 135 HA PRO A 12133.622 13.096 -1.437 1.00 0.00 H 136 1HB PRO A 12132.336 12.276 1.117 1.00 0.00 H ATOM 137 2HB PRO A 12132.579 13.893 0.447 1.00 0.00 H **ATOM ATOM** 138 1HG PRO A 12130.170 12.758 0.426 1.00 0.00 H 139 2HG PRO A 12130.728 13.741 -0.940 1.00 0.00 H ATOM **ATOM** 140 1HD PRO A 12130.539 10.770 -0.691 1.00 0.00 H 141 2HD PRO A 12130.219 11.809 -2.094 1.00 0.00 H ATOM 142 N GLY A 13134.030 10.155 -0.108 1.00 0.00 N **ATOM** 143 CA GLY A 13135.012 9.261 0.477 1.00 0.00 C **ATOM** 144 C GLY A 13135.208 7.999 -0.339 1.00 0.00 C **ATOM** 145 O GLY A 13135.145 6.891 0.193 1.00 0.00 O ATOM 146 H GLY A 13133.170 9.800 -0.417 1.00 0.00 H **ATOM** 147 1HA GLY A 13135.957 9.779 0.552 1.00 0.00 H **ATOM** 148 2HA GLY A 13134.686 8.986 1.470 1.00 0.00 H **ATOM** 149 N ASNA 14135.447 8.169 -1.638 1.00 0.00 N **ATOM** 150 CA ASN A 14135.654 7.038 -2.536 1.00 0.00 C **ATOM** 151 C ASN A 14134.405 6.163 -2.612 1.00 0.00 C **ATOM** 152 O ASN A 14133.628 6.256 -3.562 1.00 0.00 O **ATOM** 153 CB ASN A 14136.854 6.205 -2.078 1.00 0.00 C **ATOM** 154 CG ASN A 14138.169 6.936 -2.265 1.00 0.00 C **ATOM** 155 OD1 ASN A 14138.694 7.023 -3.375 1.00 0.00 O **ATOM** 156 ND2 ASN A 14138.711 7.466 -1.173 1.00 0.00 N **ATOM** 157 H ASNA 14135.485 9.078 -2.000 1.00 0.00 H ATOM 158 HA ASN A 14135.858 7.433 -3.520 1.00 0.00 H ATOM 159 1HB ASN A 14136.742 5.965 -1.032 1.00 0.00 H ATOM

160 2HB ASN A 14136.888 5.290 -2.652 1.00 0.00 H ATOM 161 1HD2 ASN A 14138.237 7.357 -0.322 1.00 0.00 H ATOM **ATOM** 162 2HD2 ASN A 14139.561 7.945 -1.264 1.00 0.00 H 163 N SER A 15134.219 5.312 -1.607 1.00 0.00 N **ATOM ATOM** 164 CA SER A 15133.065 4.422 -1.564 1.00 0.00 C 165 C SER A 15132.542 4.276 -0.139 1.00 0.00 C **ATOM ATOM** 166 O SER A 15131.340 4.379 0.107 1.00 0.00 O **ATOM** 167 CB SER A 15133.432 3.048 -2.127 1.00 0.00 C 168 OG SER A 15132.293 2.391 -2.653 1.00 0.00 O **ATOM ATOM** 169 H SER A 15134.872 5.282 -0.878 1.00 0.00 H 170 HA SER A 15132.289 4.856 -2.176 1.00 0.00 H **ATOM ATOM** 171 1HB SER A 15134.159 3.167 -2.917 1.00 0.00 H **ATOM** 172 2HB SER A 15133.853 2.439 -1.340 1.00 0.00 H 173 HG SER A 15131.783 3.007 -3.183 1.00 0.00 H **ATOM ATOM** 174 N HIS A 16133.453 4.036 0.799 1.00 0.00 N 175 CA HIS A 16133.084 3.876 2.201 1.00 0.00 C **ATOM** 176 C HIS A 16133.923 4.787 3.092 1.00 0.00 C ATOM 177 O HIS A 16133.400 5.454 3.984 1.00 0.00 O **ATOM** 178 CB HIS A 16133.259 2.420 2.633 1.00 0.00 C ATOM 179 CG HIS A 16132.025 1.591 2.457 1.00 0.00 C **ATOM** 180 ND1 HIS A 16131.474 0.835 3.472 1.00 0.00 N **ATOM** 181 CD2 HIS A 16131.232 1.401 1.377 1.00 0.00 C **ATOM** 182 CE1 HIS A 16130.397 0.216 3.023 1.00 0.00 C **ATOM** 183 NE2 HIS A 16130.227 0.543 1.755 1.00 0.00 N ATOM 184 H HIS A 16134.396 3.965 0.542 1.00 0.00 H **ATOM** 185 HA HIS A 16132.045 4.150 2.304 1.00 0.00 H ATOM 186 1HB HIS A 16134.047 1.970 2.047 1.00 0.00 H **ATOM** 187 2HB HIS A 16133.534 2.391 3.678 1.00 0.00 H **ATOM** 188 HD1 HIS A 16131.822 0.763 4.385 1.00 0.00 H **ATOM** 189 HD2 HIS A 16131.363 1.841 0.399 1.00 0.00 H ATOM 190 HE1 HIS A 16129.763 -0.444 3.596 1.00 0.00 H ATOM

191 HE2 HIS A 16129.457 0.291 1.205 1.00 0.00 H **ATOM ATOM** 192 N GLY A 17135.229 4.809 2.843 1.00 0.00 N **ATOM** 193 CA GLY A 17136.120 5.641 3.630 1.00 0.00 C 194 C GLY A 17137.532 5.092 3.679 1.00 0.00 C **ATOM** 195 O GLY A 17138.032 4.742 4.748 1.00 0.00 O **ATOM** 196 H GLYA 17135.589 4.257 2.119 1.00 0.00 H **ATOM ATOM** 197 1HA GLY A 17136.145 6.631 3.200 1.00 0.00 H 198 2HA GLY A 17135.736 5.707 4.637 1.00 0.00 H **ATOM** 199 N LEUA 18138.175 5.015 2.519 1.00 0.00 N **ATOM ATOM** 200 CA LEU A 18139.539 4.503 2.434 1.00 0.00 C ATOM 201 C LEU A 18140.547 5.574 2.836 1.00 0.00 C **ATOM** 202 O LEUA 18140.918 6.426 2.029 1.00 0.00 O 203 CB LEU A 18139.833 4.014 1.015 1.00 0.00 C ATOM 204 CG LEUA 18138.730 3.165 0.380 1.00 0.00 C ATOM 205 CD1 LEU A 18138.853 3.178 -1.136 1.00 0.00 C ATOM 206 CD2 LEU A 18138.786 1.740 0.909 1.00 0.00 C **ATOM** 207 H LEUA 18137.723 5.308 1.701 1.00 0.00 H ATOM 208 HA LEU A 18139.623 3.672 3.116 1.00 0.00 H **ATOM** 209 1HB LEU A 18140.002 4.877 0.387 1.00 0.00 H ATOM 210 2HB LEU A 18140.739 3.426 1.040 1.00 0.00 H **ATOM ATOM** 211 HG LEU A 18137.769 3.583 0.641 1.00 0.00 H **ATOM** 212 1HD1 LEU A 18139.875 2.973 -1.416 1.00 0.00 H **ATOM** 213 2HD1 LEU A 18138.564 4.149 -1.512 1.00 0.00 H 214 3HD1 LEU A 18138.205 2.423 -1.556 1.00 0.00 H ATOM 215 1HD2 LEU A 18137.874 1.224 0.648 1.00 0.00 H ATOM 216 2HD2 LEU A 18138.895 1.758 1.983 1.00 0.00 H ATOM 217 3HD2 LEU A 18139.629 1.226 0.470 1.00 0.00 H **ATOM** 218 N GLUA 19140.988 5.523 4.088 1.00 0.00 N **ATOM** 219 CA GLUA 19141.956 6.488 4.598 1.00 0.00 C ATOM 220 C GLUA 19143.006 5.799 5.464 1.00 0.00 C ATOM ATOM 221 O GLU A 19142.962 4.585 5.662 1.00 0.00 O

222 CB GLUA 19141.246 7.576 5.405 1.00 0.00 C 223 CG GLUA 19140.290 7.030 6.453 1.00 0.00 C **ATOM** 224 CD GLUA 19140.046 8.008 7.586 1.00 0.00 C **ATOM** 225 OE1 GLU A 19139.639 7.561 8.679 1.00 0.00 O **ATOM** 226 OE2 GLU A 19140.261 9.220 7.380 1.00 0.00 O ATOM 227 H GLUA 19140.656 4.819 4.684 1.00 0.00 H **ATOM** 228 HA GLU A 19142.447 6.944 3.751 1.00 0.00 H **ATOM** 229 1HB GLU A 19141.989 8.180 5.907 1.00 0.00 H **ATOM** 230 2HB GLU A 19140.683 8.202 4.728 1.00 0.00 H **ATOM** 231 1HG GLU A 19139.345 6.807 5.981 1.00 0.00 H ATOM 232 2HG GLU A 19140.708 6.122 6.864 1.00 0.00 H **ATOM** 233 N VALA 20143.949 6.582 5.978 1.00 0.00 N **ATOM** 234 CA VALA 20145.009 6.047 6.822 1.00 0.00 C ATOM 235 C VALA 20144.435 5.407 8.082 1.00 0.00 C **ATOM** 236 O VALA 20143.542 5.963 8.722 1.00 0.00 O ATOM 237 CB VALA 20146.013 7.144 7.229 1.00 0.00 C ATOM 238 CG1 VAL A 20147.191 6.540 7.979 1.00 0.00 C ATOM 239 CG2 VAL A 20146.489 7.914. 6.004 1.00 0.00 C **ATOM** 240 H VALA 20143.931 7.543 5.783 1.00 0.00 H **ATOM** 241 HA VALA 20145.539 5.294 6.257 1.00 0.00 H ATOM 242 HB VALA 20145.512 7.835 7.889 1.00 0.00 H **ATOM** 243 1HG1 VAL A 20147.488 5.618 7.501 1.00 0.00 H **ATOM** 244 2HG1 VAL A 20146.903 6.341 9.000 1.00 0.00 H **ATOM** 245 3HG1 VALA 20148.019 7.235 7.967 1.00 0.00 H ATOM 246 1HG2 VAL A 20147.486 7.592 5.743 1.00 0.00 H **ATOM** 247 2HG2 VAL A 20146.498 8.971 6.226 1.00 0.00 H ATOM 248 3HG2 VAL A 20145.821 7.726 5.177 1.00 0.00 H **ATOM** 249 N GLY A 21144.954 4.234 8.432 1.00 0.00 N ATOM 250 CA GLY A 21144.482 3.538 9.615 1.00 0.00 C ATOM 251 C GLYA 21143.450 2.476 9.287 1.00 0.00 C **ATOM** ATOM 252 O GLY A 21143.375 1.447 9.959 1.00 0.00 O

253 H GLY A 21145.665 3.840 7.885 1.00 0.00 H 254 1HA GLY A 21145.323 3.069 10.104 1.00 0.00 H **ATOM** 255 2HA GLY A 21144.039 4.256 10.290 1.00 0.00 H **ATOM ATOM** 256 N SER A 22142.655 2.725 8.253 1.00 0.00 N 257 CA SER A 22141.623 1.781 7.837 1.00 0.00 C **ATOM** 258 C SER A 22142.196 0.728 6.895 1.00 0.00 C **ATOM** 259 O SER A 22143.138 0.996 6.147 1.00 0.00 O ATOM 260 CB SER A 22140.471 2.521 7.154 1.00 0.00 C **ATOM** 261 OG SER A 22140.308 3.821 7.694 1.00 0.00 O **ATOM** 262 H SER A 22142.764 3.562 7.756 1.00 0.00 H ATOM ATOM 263 HA SER A 22141.249 1.289 8.722 1.00 0.00 H 264 1HB SER A 22140.678 2.607 6.098 1.00 0.00 H ATOM 265 2HB SER A 22139.556 1.967 7.298 1.00 0.00 H ATOM 266 HG SER A 22140.349 3.777 8.653 1.00 0.00 H ATOM ATOM 267 N LEUA 23141.624 -0.470 6.936 1.00 0.00 N 268 CA LEU A 23142.078 -1.564 6.086 1.00 0.00 C **ATOM** 269 C LEUA 23141.426 -1.492 4.709 1.00 0.00 C ATOM 270 O LEUA 23140.229 -1.231 4.590 1.00 0.00 O ATOM **ATOM** 271 CB LEU A 23141.763 -2.911 6.740 1.00 0.00 C 272 CG LEU A 23142.577 -3.225 7.997 1.00 0.00 C ATOM 273 CD1 LEU A 23141.779 -4.108 8.943 1.00 0.00 C ATOM 274 CD2 LEU A 23143.893 -3.892 7.624 1.00 0.00 C ATOM 275 H LEUA 23140.877 -0.622 7.552 1.00 0.00 H ATOM 276 HA LEU A 23143.148 -1.472 5.970 1.00 0.00 H ATOM 277 1HB LEU A 23140.716 -2.923 7.003 1.00 0.00 H **ATOM** 278 2HB LEU A 23141.945 -3.691 6.017 1.00 0.00 H ATOM 279 HG LEU A 23142.803 -2.303 8.512 1.00 0.00 H **ATOM** 280 1HD1 LEU A 23141.062 -4.686 8.378 1.00 0.00 H **ATOM** 281 2HD1 LEU A 23141.259 -3.490 9.659 1.00 0.00 H ATOM **ATOM** 282 3HD1 LEU A 23142.449 -4.777 9.464 1.00 0.00 H 283 1HD2 LEU A 23143.706 -4.908 7.309 1.00 0.00 H ATOM

- ATOM 284 2HD2 LEU A 23144.550 -3.897 8.481 1.00 0.00 H
- ATOM 285 3HD2 LEU A 23144.359 -3.345 6.818 1.00 0.00 H
- ATOM 286 N ALA A 24142.222 -1.725 3.670 1.00 0.00 N
- ATOM 287 CA ALA A 24141.724 -1.686 2.301 1.00 0.00 C
- ATOM 288 C ALA A 24142.324 -2.812 1.466 1.00 0.00 C
- ATOM 289 O ALAA 24143.420 -3.294 1.751 1.00 0.00 O
- ATOM 290 CB ALA A 24142.028 -0.337 1.667 1.00 0.00 C
- ATOM 291 H ALA A 24143.168 -1.928 3.829 1.00 0.00 H
- ATOM 292 HA ALA A 24140.651 -1.808 2.334 1.00 0.00 H
- ATOM 293 1HB ALA A 24141.196 0.333 1.830 1.00 0.00 H
- ATOM 294 2HB ALA A 24142.184 -0.464 0.606 1.00 0.00 H
- ATOM 295 3HB ALA A 24142.919 0.079 2.115 1.00 0.00 H
- ATOM 296 N GLU A 25141.598 -3.227 0.433 1.00 0.00 N
- ATOM 297 CA GLU A 25142.059 -4.299 -0.445 1.00 0.00 C
- ATOM 298 C GLU A 25142.225 -3.797 -1.876 1.00 0.00 C
- ATOM 299 O GLUA 25141.447 -2.968 -2.348 1.00 0.00 O
- ATOM 300 CB GLU A 25141.075 -5.470 -0.414 1.00 0.00 C
- ATOM 301 CG GLU A 25141.514 -6.654 -1.260 1.00 0.00 C
- ATOM 302 CD GLU A 25140.767 -6.737 -2.578 1.00 0.00 C
- ATOM 303 OE1 GLU A 25140.490 -5.674 -3.170 1.00 0.00 O
- ATOM 304 OE2 GLU A 25140.461 -7.865 -3.017 1.00 0.00 O
- ATOM 305 H GLUA 25140.732 -2.805 0.256 1.00 0.00 H
- ATOM 306 HA GLU A 25143.017 -4.636 -0.081 1.00 0.00 H
- ATOM 307 1HB GLU A 25140.965 -5.805 0.607 1.00 0.00 H
- ATOM 308 2HB GLU A 25140.117 -5.130 -0.778 1.00 0.00 H
- ATOM 309 1HG GLUA 25142.569 -6.561 -1.469 1.00 0.00 H
- ATOM 310 2HG GLU A 25141.335 -7.563 -0.704 1.00 0.00 H
- ATOM 311 N VALA 26143.244 -4.305 -2.560 1.00 0.00 N
- ATOM 312 CA VALA 26143.513 -3.909 -3.937 1.00 0.00 C
- ATOM 313 C VALA 26142.949 -4.926 -4.922 1.00 0.00 C
- ATOM 314 O VALA 26142.719 -6.084 -4.571 1.00 0.00 O

- ATOM 315 CB VALA 26145.024 -3.751 -4.191 1.00 0.00 C ATOM 316 CG1 VALA 26145.275 -3.136 -5.559 1.00 0.00 C
- ATOM 317 CG2 VAL A 26145.665 -2.911 -3.097 1.00 0.00 C
- ATOM 318 H VALA 26143.830 -4.962 -2.129 1.00 0.00 H
- ATOM 319 HA VALA 26143.039 -2.953 -4.109 1.00 0.00 H
- ATOM 320 HB VALA 26145.477 -4.731 -4.173 1.00 0.00 H
- ATOM 321 1HG1 VAL A 26146.222 -2.616 -5.553 1.00 0.00 H
- ATOM 322 2HG1 VAL A 26144.484 -2.439 -5.792 1.00 0.00 H
- ATOM 323 3HG1 VAL A 26145.299 -3.917 -6.305 1.00 0.00 H
- ATOM 324 1HG2 VAL A 26145.381 -1.876 -3.223 1.00 0.00 H
- ATOM 325 2HG2 VAL A 26146.740 -2.998 -3.157 1.00 0.00 H
- ATOM 326 3HG2 VAL A 26145.330 -3.260 -2.131 1.00 0.00 H
- ATOM 327 N LYS A 27142.727 -4.487 -6.157 1.00 0.00 N
- ATOM 328 CA LYS A 27142.188 -5.360 -7.194 1.00 0.00 C
- ATOM 329 C LYS A 27143.310 -5.966 -8.031 1.00 0.00 C
- ATOM 330 O LYS A 27143.259 -5.951 -9.262 1.00 0.00 O
- ATOM 331 CB LYS A 27141.223 -4.583 -8.092 1.00 0.00 C
- ATOM 332 CG LYS A 27139.924 -4.202 -7.403 1.00 0.00 C
- ATOM 333 CD LYS A 27139.048 -5.419 -7.154 1.00 0.00 C
- ATOM 334 CE LYS A 27137.646 -5.018 -6.724 1.00 0.00 C
- ATOM 335 NZ LYS A 27137.102 -5.932 -5.682 1.00 0.00 N
- ATOM 336 H LYS A 27142.930 -3.554 -6.376 1.00 0.00 H
- ATOM 337 HA LYS A 27141.648 -6.158 -6.706 1.00 0.00 H
- ATOM 338 1HB LYS A 27141.710 -3.677 -8.424 1.00 0.00 H
- ATOM 339 2HB LYS A 27140.985 -5.190 -8.954 1.00 0.00 H
- ATOM 340 1HG LYS A 27140.152 -3.735 -6.457 1.00 0.00 H
- ATOM 341 2HG LYS A 27139.387 -3.504 -8.030 1.00 0.00 H
- ATOM 342 1HD LYS A 27138.983 -5.995 -8.065 1.00 0.00 H
- ATOM 343 2HD LYS A 27139.496 -6.019 -6.376 1.00 0.00 H
- ATOM 344 1HE LYS A 27137.678 -4.014 -6.327 1.00 0.00 H
- ATOM 345 2HE LYS A 27136.998 -5.043 -7.587 1.00 0.00 H

346 1HZ LYS A 27136.733 -6.799 -6.124 1.00 0.00 H ATOM **ATOM** 347 2HZ LYS A 27136.331 -5.466 -5.163 1.00 0.00 H 348 3HZ LYS A 27137.851 -6.192 -5.007 1.00 0.00 H ATOM **ATOM** 349 N GLUA 28144.323 -6.501 -7.357 1.00 0.00 N 350 CA GLUA 28145.457 -7.112 -8.038 1.00 0.00 C **ATOM** 351 C GLUA 28145.269 -8.622 -8.160 1.00 0.00 C ATOM **ATOM** 352 O GLUA 28144.303 -9.181 -7.640 1.00 0.00 O **ATOM** 353 CB GLU A 28146.756 -6.806 -7.288 1.00 0.00 C **ATOM** 354 CG GLU A 28147.863 -6.272 -8.182 1.00 0.00 C 355 CD GLUA 28149.224 -6.837 -7.824 1.00 0.00 C **ATOM ATOM** 356 OE1 GLU A 28149.635 -7.835 -8.452 1.00 0.00 O **ATOM** 357 OE2 GLU A 28149.878 -6.281 -6.917 1.00 0.00 O **ATOM** 358 H GLUA 28144.307 -6.483 -6.377 1.00 0.00 H 359 HA GLUA 28145.516 -6.688 -9.029 1.00 0.00 H **ATOM** 360 1HB GLU A 28146.552 -6.068 -6.526 1.00 0.00 H **ATOM** 361 2HB GLU A 28147.110 -7.711 -6.814 1.00 0.00 H **ATOM** 362 1HG GLU A 28147.640 -6.533 -9.205 1.00 0.00 H **ATOM** ATOM 363 2HG GLU A 28147.899 -5.197 -8.085 1.00 0.00 H 364 N ASNA 29146.199 -9.275 -8.850 1.00 0.00 N ATOM 365 CA ASN A 29146.136 -10.719 -9.040 1.00 0.00 C **ATOM** 366 C ASN A 29146.156 -11.446 -7.697 1.00 0.00 C **ATOM** 367 O ASN A 29145.239 -12.204 -7.381 1.00 0.00 O ATOM 368 CB ASN A 29147.306 -11.191 -9.907 1.00 0.00 C **ATOM ATOM** 369 CG ASN A 29146.930 -11.306 -11.371 1.00 0.00 C 370 OD1 ASN A 29146.786 -12.407 -11.903 1.00 0.00 O ATOM 371 ND2 ASN A 29146.767 -10.165 -12.032 1.00 0.00 N **ATOM** 372 H ASN A 29146.944 -8.773 -9.240 1.00 0.00 H ATOM 373 HA ASN A 29145.211 -10.947 -9.546 1.00 0.00 H **ATOM** 374 1HB ASN A 29148.119 -10.486 -9.819 1.00 0.00 H ATOM 375 2HB ASN A 29147.635 -12.160 -9.561 1.00 0.00 H ATOM: 376 1HD2 ASN A 29146.898 -9.325 -11.543 1.00 0.00 H ATOM

- ATOM 377 2HD2 ASN A 29146.524 -10.210 -12.979 1.00 0.00 H
- ATOM 378 N PRO A 30147.206 -11.226 -6.887 1.00 0.00 N
- ATOM 379 CA PRO A 30147.337 -11.863 -5.575 1.00 0.00 C
- ATOM 380 C PRO A 30146.420 -11.233 -4.529 1.00 0.00 C
- ATOM 381 O PRO A 30146.641 -10.098 -4.105 1.00 0.00 O
- ATOM 382 CB PRO A 30148.802 -11.621 -5.217 1.00 0.00 C
- ATOM 383 CG PRO A 30149.156 -10.354 -5.917 1.00 0.00 C
- ATOM 384 CD PRO A 30148.346 -10.336 -7.187 1.00 0.00 C
- ATOM 385 HA PRO A 30147.149 -12.925 -5.631 1.00 0.00 H
- ATOM 386 1HB PRO A 30148.902 -11.522 -4.145 1.00 0.00 H
- ATOM 387 2HB PRO A 30149.404 -12.446 -5.567 1.00 0.00 H
- ATOM 388 1HG PRO A 30148.897 -9.508 -5.296 1.00 0.00 H
- ATOM 389 2HG PRO A 30150.211 -10.344 -6.145 1.00 0.00 H
- ATOM 390 1HD PRO A 30148.006 -9.335 -7.401 1.00 0.00 H
- ATOM 391 2HD PRO A 30148.927 -10.721 -8.009 1.00 0.00 H
- ATOM 392 N PRO A 31145.373 -11.959 -4.095 1.00 0.00 N
- ATOM 393 CA PRO A 31144.428 -11.455 -3.094 1.00 0.00 C
- ATOM 394 C PRO A 31145.065 -11.310 -1.717 1.00 0.00 C
- ATOM 395 O PRO A 31144.943 -12.193 -0.869 1.00 0.00 O
- ATOM 396 CB PRO A 31143.331 -12.523 -3.065 1.00 0.00 C
- ATOM 397 CG PRO A 31143.999 -13.765 -3.541 1.00 0.00 C
- ATOM 398 CD PRO A 31145.028 -13.322 -4.543 1.00 0.00 C
- ATOM 399 HA PRO A 31144.003 -10.507 -3.393 1.00 0.00 H
- ATOM 400 1HB PRO A 31142.960 -12.634 -2.057 1.00 0.00 H
- ATOM 401 2HB PRO A 31142.524 -12.233 -3.721 1.00 0.00 H
- ATOM 402 1HG PRO A 31144.474 -14.268 -2.712 1.00 0.00 H
- ATOM 403 2HG PRO A 31143.276 -14.415 -4.011 1.00 0.00 H
- ATOM 404 1HD PRO A 31145.892 -13.969 -4.508 1.00 0.00 H
- ATOM 405 2HD PRO A 31144.607 -13.306 -5.536 1.00 0.00 H
- ATOM 406 N PHE A 32145.746 -10.189 -1.501 1.00 0.00 N
- ATOM 407 CA PHE A 32146.404 -9.928 -0.226 1.00 0.00 C

408 C PHE A 32145.573 -8.975 0.628 1.00 0.00 C **ATOM** 409 O PHE A 32144.568 -8.432 0.172 1.00 0.00 O **ATOM ATOM** 410 CB PHE A 32147.798 -9.342 -0.457 1.00 0.00 C 411 CG PHE A 32147.825 -8.245 -1.484 1.00 0.00 C **ATOM** 412 CD1 PHE A 32147.160 -7.051 -1.259 1.00 0.00 C **ATOM ATOM** 413 CD2 PHE A 32148.516 -8.409 -2.674 1.00 0.00 C ATOM 414 CE1 PHE A 32147.184 -6.040 -2.201 1.00 0.00 C ATOM 415 CE2 PHE A 32148.543 -7.402 -3.620 1.00 0.00 C **ATOM** 416 CZ PHE A 32147.875 -6.216 -3.383 1.00 0.00 C 417 H PHE A 32145.807 -9.522 -2.217 1.00 0.00 H ATOM **ATOM** 418 HA PHE A 32146.501 -10.868 0.295 1.00 0.00 H ATOM 419 1HB PHE A 32148.168 -8.935 0.471 1.00 0.00 H ATOM 420 2HB PHE A 32148.460 -10.127 -0.791 1.00 0.00 H **ATOM** 421 HD1 PHE A 32146.618 -6.912 -0.335 1.00 0.00 H **ATOM** 422 HD2 PHE A 32149.038 -9.336 -2.860 1.00 0.00 H **ATOM** 423 HE1 PHE A 32146.660 -5.114 -2.014 1.00 0.00 H 424 HE2 PHE A 32149.085 -7.543 -4.543 1.00 0.00 H ATOM **ATOM** 425 HZ PHE A 32147.895 -5.428 -4.122 1.00 0.00 H ATOM 426 N TYR A 33146.003 -8.777 1.870 1.00 0.00 N 427 CA TYR A 33145.297 -7.889 2.789 1.00 0.00 C **ATOM** 428 C TYR A 33146.273 -6.965 3.508 1.00 0.00 C ATOM 429 O TYR A 33147.259 -7.417 4.092 1.00 0.00 O **ATOM** ATOM 430 CB TYR A 33144.502 -8.706 3.809 1.00 0.00 C **ATOM** 431 CG TYR A 33143.206 -9.261 3.263 1.00 0.00 C 432 CD1 TYR A 33142.351 -8.466 2.509 1.00 0.00 C ATOM 433 CD2 TYR A 33142.838 -10.579 3.501 1.00 0.00 C **ATOM ATOM** 434 CE1 TYR A 33141.165 -8.970 2.008 1.00 0.00 C 435 CE2 TYR A 33141.655 -11.090 3.002 1.00 0.00 C ATOM ATOM 436 CZ TYR A 33140.822 -10.282 2.257 1.00 0.00 C 437 OH TYR A 33139.643 -10.787 1.759 1.00 0.00 O **ATOM** 438 H TYR A 33146.811 -9.238 2.178 1.00 0.00 H ATOM

439 HA TYR A 33144.613 -7.289 2.208 1.00 0.00 H 440 1HB TYR A 33145.104 -9.537 4.143 1.00 0.00 H ATOM 441 2HB TYR A 33144.264 -8.077 4.655 1.00 0.00 H **ATOM** 442 HD1 TYR A 33142.623 -7.439 2.316 1.00 0.00 H ATOM 443 HD2 TYR A 33143.492 -11.209 4.086 1.00 0.00 H ATOM ATOM 444 HE1 TYR A 33140.515 -8.336 1.424 1.00 0.00 H 445 HE2 TYR A 33141.386 -12.117 3.198 1.00 0.00 H ATOM 446 HH TYR A 33139.504 -10.457 0.869 1.00 0.00 H **ATOM** 447 N GLY A 34145.993 -5.666 3.463 1.00 0.00 N ATOM 448 CA GLY A 34146.856 -4.698 4.115 1.00 0.00 C **ATOM** 449 C GLY A 34146.086 -3.512 4.663 1.00 0.00 C **ATOM** 450 O GLY A 34144.877 -3.403 4.464 1.00 0.00 O ATOM 451 H GLY A 34145.194 -5.363 2.983 1.00 0.00 H ATOM 452 1HA GLY A 34147.374 -5.184 4.928 1.00 0.00 H **ATOM** 453 2HA GLY A 34147.583 -4.342 3.400 1.00 0.00 H **ATOM** 454 N VALA 35146.789 -2.622 5.357 1.00 0.00 N **ATOM** 455 CA VALA 35146.165 -1.439 5.937 1.00 0.00 C ATOM 456 C VALA 35146.791 -0.162 5.382 1.00 0.00 C ATOM 457 O VALA 35147.999 -0.097 5.159 1.00 0.00 O **ATOM** 458 CB VALA 35146.287 -1.437 7.474 1.00 0.00 C ATOM 459 CG1 VAL A 35147.746 -1.405 7.899 1.00 0.00 C **ATOM** 460 CG2 VAL A 35145.523 -0.263 8.071 1.00 0.00 C ATOM 461 H VALA 35147.751 -2.766 5.482 1.00 0.00 H ATOM 462 HA VALA 35145.116 -1.455 5.679 1.00 0.00 H ATOM 463 HB VALA 35145.847 -2.350 7.849 1.00 0.00 H ATOM 464 1HG1 VAL A 35148.023 -0.395 8.165 1.00 0.00 H ATOM 465 2HG1 VAL A 35148.367 -1.745 7.084 1.00 0.00 H ATOM 466 3HG1 VAL A 35147.888 -2.052 8.752 1.00 0.00 H **ATOM** 467 1HG2 VAL A 35144.502 -0.284 7.721 1.00 0.00 H ATOM 468 2HG2 VAL A 35145.989 0.662 7.765 1.00 0.00 H **ATOM** 469 3HG2 VAL A 35145.537 -0.335 9.148 1.00 0.00 H

470 N ILE A 36145.958 0.852 5.164 1.00 0.00 N ATOM **ATOM** 471 CA ILE A 36146.430 2.126 4.637 1.00 0.00 C 472 C ILE A 36147.393 2.798 5.611 1.00 0.00 C **ATOM** 473 O ILE A 36147.154 2.821 6.819 1.00 0.00 O ATOM 474 CB ILE A 36145.259 3.085 4.344 1.00 0.00 C **ATOM** 475 CG1 ILE A 36144.203 2.391 3.480 1.00 0.00 C **ATOM** 476 CG2 ILE A 36145.765 4.346 3.658 1.00 0.00 C **ATOM** 477 CD1 ILE A 36143.021 3.272 3.144 1.00 0.00 C **ATOM** 478 H ILEA 36145.006 0.739 5.363 1.00 0.00 H **ATOM** 479 HA ILE A 36146.950 1.932 3.710 1.00 0.00 H **ATOM** 480 HB ILE A 36144.813 3.371 5.284 1.00 0.00 H ATOM 481 1HG1 ILE A 36144.657 2.077 2.552 1.00 0.00 H **ATOM** 482 2HG1 ILE A 36143.832 1.522 4.005 1.00 0.00 H ATOM 483 1HG2 ILE A 36144.985 5.093 3.655 1.00 0.00 H · ATOM 484 2HG2 ILE A 36146.045 4.115 2.640 1.00 0.00 H ATOM 485 3HG2 ILE A 36146.625 4.726 4.190 1.00 0.00 H **ATOM** 486 1HD1 ILE A 36143.302 4.309 3.253 1.00 0.00 H ATOM 487 2HD1 ILE A 36142.203 3.047 3.812 1.00 0.00 H ATOM 488 3HD1 ILE A 36142.713 3.089 2.125 1.00 0.00 H ATOM 489 N ARG A 37148.482 3.342 5.078 1.00 0.00 N ATOM 490 CA ARG A 37149.482 4.013 5.901 1.00 0.00 C **ATOM** 491 C ARG A 37149.654 5.467 5.474 1.00 0.00 C ATOM 492 O ARG A 37149.380 6.387 6.245 1.00 0.00 O **ATOM** 493 CB ARG A 37150.821 3.279 5.811 1.00 0.00 C **ATOM** 494 CG ARG A 37150.720 1.790 6.099 1.00 0.00 C **ATOM** 495 CD ARG A 37150.093 1.526 7.458 1.00 0.00 C ATOM 496 NE ARG A 37150.689 2.353 8.506 1.00 0.00 N ATOM 497 CZ ARG A 37150.129 2.558 9.696 1.00 0.00 C ATOM 498 NH1 ARG A 37148.963 1.999 9.993 1.00 0.00 N ATOM 499 NH2 ARG A 37150.737 3.323 10.591 1.00 0.00 N ATOM 500 H ARG A 37148.617 3.291 4.109 1.00 0.00 H ATOM

501 HA ARG A 37149.138 3.991 6.924 1.00 0.00 H **ATOM** 502 1HB ARG A 37151.221 3.405 4.816 1.00 0.00 H **ATOM** ATOM 503 2HB ARG A 37151.507 3.716 6.522 1.00 0.00 H 504 1HG ARG A 37150.112 1.327 5.337 1.00 0.00 H ATOM 505 2HG ARG A 37151.712 1.362 6.079 1.00 0.00 H ATOM 506 1HD ARG A 37149.036 1.741 7.401 1.00 0.00 H ATOM 507 2HD ARG A 37150.235 0.486 7.710 1.00 0.00 H ATOM 508 HE ARG A 37151.550 2.778 8.311 1.00 0.00 H **ATOM** 509 1HH1 ARG A 37148.498 1.422 9.322 1.00 0.00 H ATOM 510 2HH1 ARG A 37148.547 2.158 10.889 1.00 0.00 H ATOM 511 1HH2 ARG A 37151.617 3.746 10.372 1.00 0.00 H ATOM 512 2HH2 ARG A 37150.318 3.477 11.485 1.00 0.00 H ATOM 513 N TRPA 38150.112 5.667 4.242 1.00 0.00 N ATOM 514 CA TRP A 38150.321 7.011 3.714 1.00 0.00 C ATOM 515 C TRPA 38149.551 7.213 2.412 1.00 0.00 C ATOM 516 O TRPA 38149.601 6.374 1.511 1.00 0.00 O **ATOM** 517 CB TRP A 38151.814 7.269 3.486 1.00 0.00 C **ATOM** 518 CG TRP A 38152.095 8.525 2.714 1.00 0.00 C ATOM 519 CD1 TRP A 38152.313 9.772 3.226 1.00 0.00 C **ATOM** 520 CD2 TRP A 38152.181 8.655 1.290 1.00 0.00 C ATOM 521 NE1 TRP A 38152.531 10.669 2.207 1.00 0.00 N **ATOM** 522 CE2 TRP A 38152.455 10.006 1.009 1.00 0.00 C **ATOM** 523 CE3 TRP A 38152.055 7.758 0.225 1.00 0.00 C **ATOM** 524 CZ2 TRP A 38152.603 10.481 -0.292 1.00 0.00 C **ATOM** 525 CZ3 TRP A 38152.202 8.230 -1.066 1.00 0.00 C ATOM 526 CH2 TRP A 38152.474 9.581 -1.315 1.00 0.00 C **ATOM** 527 H TRPA 38150.313 4.895 3.674 1.00 0.00 H ATOM 528 HA TRP A 38149.952 7.715 4.446 1.00 0.00 H ATOM 529 1HB TRP A 38152.309 7.350 4.443 1.00 0.00 H ATOM 530 2HB TRP A 38152.236 6.439 2.938 1.00 0.00 H **ATOM** 531 HD1 TRP A 38152.312 10.006 4.280 1.00 0.00 H

532 HE1 TRP A 38152.711 11.625 2.319 1.00 0.00 H 533 HE3 TRP A 38151.845 6.713 0.397 1.00 0.00 H ATOM 534 HZ2 TRP A 38152.809 11.521 -0.501 1.00 0.00 H ATOM 535 HZ3 TRP A 38152.108 7.552 -1.900 1.00 0.00 H ATOM ATOM 536 HH2 TRP A 38152.582 9.906 -2.340 1.00 0.00 H ATOM 537 N ILE A 39148.850 8.337 2.318 1.00 0.00 N 538 CA ILE A 39148.078 8.664 1.126 1.00 0.00 C ATOM 539 C ILE A 39148.492 10.024 0.575 1.00 0.00 C ATOM 540 O ILE A 39148.159 11.062 1.146 1.00 0.00 O **ATOM ATOM** 541 CB ILE A 39146.566 8.679 1.420 1.00 0.00 C **ATOM** 542 CG1 ILE A 39146.151 7.396 2.143 1.00 0.00 C 543 CG2 ILE A 39145.777 8.844 0.129 1.00 0.00 C ATOM 544 CD1 ILE A 39144.691 7.371 2.539 1.00 0.00 C **ATOM** 545 H ILE A 39148.859 8.968 3.067 1.00 0.00 H **ATOM ATOM** 546 HA ILE A 39148.275 7.907 0.380 1.00 0.00 H 547 HB ILE A 39146.353 9.526 2.053 1.00 0.00 H **ATOM** 548 1HG1 ILE A 39146.334 6.551 1.496 1.00 0.00 H **ATOM** 549 2HG1 ILE A 39146.742 7.290 3.041 1.00 0.00 H ATOM 550 1HG2 ILE A 39144.765 8.499 0.279 1.00 0.00 H **ATOM** 551 2HG2 ILE A 39146.242 8.264 -0.654 1.00 0.00 H ATOM 552 3HG2 ILE A 39145.764 9.886 -0.154 1.00 0.00 H **ATOM** 553 1HD1 ILE A 39144.182 8.211 2.090 1.00 0.00 H **ATOM** 554 2HD1 ILE A 39144.608 7.431 3.614 1.00 0.00 H **ATOM** 555 3HD1 ILE A 39144.241 6.451 2.194 1.00 0.00 H **ATOM** 556 N GLY A 40149.226 10.012 -0.532 1.00 0.00 N ATOM 557 CA GLY A 40149.678 11.253 -1.131 1.00 0.00 C ATOM 558 C GLY A 40150.185 11.072 -2.546 1.00 0.00 C ATOM 559 O GLY A 40150.020 10.007 -3.142 1.00 0.00 O ATOM 560 H GLY A 40149.467 9.155 -0.943 1.00 0.00 H ATOM **ATOM** 561 1HA GLY A 40148.858 11.955 -1.141 1.00 0.00 H 562 2HA GLY A 40150.474 11.659 -0.526 1.00 0.00 H ATOM

563 N GLN A 41150.799 12.118 -3.087 1.00 0.00 N **ATOM** 564 CA GLN A 41151.332 12.082 -4.441 1.00 0.00 C **ATOM** 565 C GLN A 41152.794 12.528 -4.460 1.00 0.00 C **ATOM** 566 O GLN A 41153.100 13.680 -4.154 1.00 0.00 O ATOM ATOM 567 CB GLN A 41150.498 12.981 -5.353 1.00 0.00 C ATOM 568 CG GLN A 41149.001 12.756 -5.223 1.00 0.00 C 569 CD GLN A 41148.213 14.050 -5.269 1.00 0.00 C ATOM 570 OE1 GLN A 41148.200 14.818 -4.307 1.00 0.00 O **ATOM** 571 NE2 GLN A 41147.549 14.296 -6.391 1.00 0.00 N **ATOM** 572 H GLNA 41150.896 12.939 -2.561 1.00 0.00 H **ATOM** 573 HA GLN A 41151.268 11.065 -4.798 1.00 0.00 H **ATOM** 574 1HB GLN A 41150.707 14.011 -5.111 1.00 0.00 H ATOM 575 2HB GLN A 41150.782 12.797 -6.377 1.00 0.00 H **ATOM** 576 1HG GLN A 41148.673 12.124 -6.034 1.00 0.00 H **ATOM** 577 2HG GLN A 41148.803 12.265 -4.282 1.00 0.00 H ATOM 578 1HE2 GLN A 41147.606 13.638 -7.115 1.00 0.00 H **ATOM** 579 2HE2 GLN A 41147.032 15.126 -6.451 1.00 0.00 H ATOM 580 N PRO A 42153.720 11.620 -4.817 1.00 0.00 N ATOM 581 CA PRO A 42155.153 11.933 -4.868 1.00 0.00 C ATOM 582 C PRO A 42155.457 13.100 -5.803 1.00 0.00 C ATOM 583 O PRO A 42154.658 13.428 -6.681 1.00 0.00 O ATOM 584 CB PRO A 42155.789 10.645 -5.399 1.00 0.00 C ATOM 585 CG PRO A 42154.802 9.575 -5.083 1.00 0.00 C **ATOM** 586 CD PRO A 42153.453 10.221 -5.197 1.00 0.00 C **ATOM** 587 HA PRO A 42155.544 12.152 -3.885 1.00 0.00 H ATOM 588 1HB PRO A 42155.950 10.733 -6.465 1.00 0.00 H ATOM 589 2HB PRO A 42156.731 10.472 -4.900 1.00 0.00 H ATOM 590 1HG PRO A 42154.894 8.767 -5.794 1.00 0.00 H ATOM 591 2HG PRO A 42154.961 9.213 -4.078 1.00 0.00 H ATOM **ATOM** 592 1HD PRO A 42153.088 10.159 -6.213 1.00 0.00 H 593 2HD PRO A 42152.754 9.763 -4.513 1.00 0.00 H ATOM

ATOM 594 N PRO A 43156.621 13.746 -5.625 1.00 0.00 N 595 CA PRO A 43157.028 14.881 -6.457 1.00 0.00 C **ATOM** 596 C PRO A 43157.418 14.454 -7.866 1.00 0.00 C ATOM ATOM 597 O PRO A 43158.590 14.200 -8.146 1.00 0.00 O 598 CB PRO A 43158.241 15.445 -5.719 1.00 0.00 C **ATOM** 599 CG PRO A 43158.803 14.285 -4.973 1.00 0.00 C ATOM 600 CD PRO A 43157.630 13.420 -4.600 1.00 0.00 C ATOM **ATOM** 601 HA PRO A 43156.254 15.632 -6.510 1.00 0.00 H 602 1HB PRO A 43158.948 15.836 -6.435 1.00 0.00 H ATOM 603 2HB PRO A 43157.926 16.230 -5.048 1.00 0.00 H ATOM 604 1HG PRO A 43159.487 13.738 -5.607 1.00 0.00 H ATOM 605 2HG PRO A 43159.311 14.631 -4.085 1.00 0.00 H **ATOM** 606 1HD PRO A 43157.903 12.376 -4.647 1.00 0.00 H ATOM 607 2HD PRO A 43157.273 13.673 -3.614 1.00 0.00 H ATOM ATOM 608 N GLY A 44156.432 14.379 -8.752 1.00 0.00 N 609 CA GLY A 44156.696 13.984 -10.122 1.00 0.00 C ATOM 610 C GLY A 44155.463 13.450 -10.820 1.00 0.00 C ATOM 611 O GLY A 44155.131 13.883 -11.924 1.00 0.00 O ATOM 612 H GLYA 44155.517 14.595 -8.473 1.00 0.00 H **ATOM** 613 1HA GLY A 44157.062 14.839 -10.667 1.00 0.00 H **ATOM** 614 2HA GLY A 44157.457 13.216 -10.121 1.00 0.00 H **ATOM** 615 N LEUA 45154.782 12.507 -10.178 1.00 0.00 N **ATOM** 616 CA LEU A 45153.577 11.916 -10.749 1.00 0.00 C **ATOM** 617 C LEUA 45152.383 12.121 -9.826 1.00 0.00 C ATOM 618 O LEUA 45152.330 11.557 -8.733 1.00 0.00 O ATOM 619 CB LEU A 45153.789 10.422 -11.006 1.00 0.00 C ATOM 620 CG LEUA 45154.407 9.647 -9.841 1.00 0.00 C **ATOM** 621 CD1 LEU A 45154.115 8.159 -9.974 1.00 0.00 C **ATOM** 622 CD2 LEU A 45155.907 9.898 -9.771 1.00 0.00 C **ATOM** 623 H LEU A 45155.095 12.205 -9.298 1.00 0.00 H ATOM 624 HA LEU A 45153.380 12.409 -11.690 1.00 0.00 H ATOM

- ATOM 625 1HB LEU A 45152.830 9.980 -11.238 1.00 0.00 H
- ATOM 626 2HB LEU A 45154.434 10.314 -11.865 1.00 0.00 H
- ATOM 627 HG LEU A 45153.966 9.991 -8.916 1.00 0.00 H
- ATOM 628 1HD1 LEU A 45155.036 7.624 -10.154 1.00 0.00 H
- ATOM 629 2HD1 LEU A 45153.438 7.995 -10.800 1.00 0.00 H
- ATOM 630 3HD1 LEU A 45153.663 7.798 -9.062 1.00 0.00 H
- ATOM 631 1HD2 LEU A 45156.426 8.959 -9.648 1.00 0.00 H
- ATOM 632 2HD2 LEU A 45156.125 10.542 -8.932 1.00 0.00 H
- ATOM 633 3HD2 LEU A 45156.236 10.374 -10.684 1.00 0.00 H
- ATOM 634 N ASNA 46151.424 12.927 -10.269 1.00 0.00 N
- ATOM 635 CA ASN A 46150.235 13.193 -9.470 1.00 0.00 C
- ATOM 636 C ASN A 46149.317 11.976 -9.459 1.00 0.00 C
- ATOM 637 O ASN A 46148.674 11.660 -10.460 1.00 0.00 O
- ATOM 638 CB ASN A 46149.488 14.408 -10.023 1.00 0.00 C
- ATOM 639 CG ASN A 46148.414 14.909 -9.078 1.00 0.00 C
- ATOM 640 OD1 ASN A 46147.337 14.320 -8.976 1.00 0.00 O
- ATOM 641 ND2 ASN A 46148.701 16.002 -8.381 1.00 0.00 N
- ATOM 642 H ASN A 46151.517 13.350 -11.148 1.00 0.00 H
- ATOM 643 HA ASN A 46150.552 13.403 -8.459 1.00 0.00 H
- ATOM 644 1HB ASN A 46150.192 15.210 -10.193 1.00 0.00 H
- ATOM 645 2HB ASN A 46149.022 14.140 -10.960 1.00 0.00 H
- ATOM 646 1HD2 ASN A 46149.578 16.418 -8.513 1.00 0.00 H
- ATOM 647 2HD2 ASN A 46148.024 16.347 -7.762 1.00 0.00 H
- ATOM 648 N GLUA 47149.262 11.298 -8.318 1.00 0.00 N
- ATOM 649 CA GLU A 47148.424 10.115 -8.169 1.00 0.00 C
- ATOM 650 C GLU A 47148.293 9.726 -6.701 1.00 0.00 C
- ATOM 651 O GLU A 47149.290 9.450 -6.033 1.00 0.00 O
- ATOM 652 CB GLU A 47149.005 8.945 -8.967 1.00 0.00 C
- ATOM 653 CG GLU A 47150.523 8.861 -8.914 1.00 0.00 C
- ATOM 654 CD GLUA 47151.092 7.924 -9.962 1.00 0.00 C
- ATOM 655 OE1 GLU A 47151.464 6.787 -9.603 1.00 0.00 O

- ATOM 656 OE2 GLU A 47151.164 8.328 -11.142 1.00 0.00 O
- ATOM 657 H GLUA 47149.799 11.601 -7.558 1.00 0.00 H
- ATOM 658 HA GLU A 47147.445 10.351 -8.555 1.00 0.00 H
- ATOM 659 1HB GLU A 47148.602 8.022 -8.577 1.00 0.00 H
- ATOM 660 2HB GLU A 47148.709 9.048 -10.001 1.00 0.00 H
- ATOM 661 1HG GLU A 47150.931 9.847 -9.076 1.00 0.00 H
- ATOM 662 2HG GLU A 47150.820 8.507 -7.938 1.00 0.00 H
- ATOM 663 N VALA 48147.064 9.696 -6.203 1.00 0.00 N
- ATOM 664 CA VALA 48146.817 9.330 -4.815 1.00 0.00 C
- ATOM 665 C VALA 48147.192 7.874 -4.570 1.00 0.00 C
- ATOM 666 O VALA 48146.430 6.963 -4.895 1.00 0.00 O
- ATOM 667 CB VALA 48145.342 9.544 -4.426 1.00 0.00 C
- ATOM 668 CG1 VAL A 48145.152 9.357 -2.928 1.00 0.00 C
- ATOM 669 CG2 VAL A 48144.869 10.922 -4.863 1.00 0.00 C
- ATOM 670 H VALA 48146.305 9.918 -6.782 1.00 0.00 H
- ATOM 671 HA VALA 48147.433 9.961 -4.188 1.00 0.00 H
- ATOM 672 HB VALA 48144.745 8.803 -4.936 1.00 0.00 H
- ATOM 673 1HG1 VAL A 48144.216 9.803 -2.627 1.00 0.00 H
- ATOM 674 2HG1 VAL A 48145.964 9.833 -2.401 1.00 0.00 H
- ATOM 675 3HG1 VAL A 48145.140 8.302 -2.696 1.00 0.00 H
- ATOM 676 1HG2 VAL A 48145.632 11.653 -4.636 1.00 0.00 H
- ATOM 677 2HG2 VAL A 48143.961 11.174 -4.337 1.00 0.00 H
- ATOM 678 3HG2 VAL A 48144.681 10.918 -5.926 1.00 0.00 H
- ATOM 679 N LEUA 49148.373 7.660 -4.000 1.00 0.00 N
- ATOM 680 CA LEU A 49148.852 6.313 -3.717 1.00 0.00 C
- ATOM 681 C LEUA 49148.792 6.021 -2.223 1.00 0.00 C
- ATOM 682 O LEUA 49149.500 6.641 -1.431 1.00 0.00 O
- ATOM 683 CB LEU A 49150.283 6.140 -4.227 1.00 0.00 C
- ATOM 684 CG LEU A 49150.454 6.288 -5.740 1.00 0.00 C
- ATOM 685 CD1 LEU A 49151.838 6.822 -6.071 1.00 0.00 C
- ATOM 686 CD2 LEU A 49150.214 4.956 -6.434 1.00 0.00 C

687 H LEUA 49148.937 8.425 -3.765 1.00 0.00 H 688 HA LEUA 49148.208 5.617 -4.234 1.00 0.00 H ATOM 689 1HB LEUA 49150.907 6.878 -3.741 1.00 0.00 H ATOM 690 2HB LEU A 49150.629 5.158 -3.942 1.00 0.00 H ATOM ATOM 691 HG LEUA 49149.726 6.995 -6.111 1.00 0.00 H ATOM 692 1HD1 LEU A 49151.800 7.900 -6.146 1.00 0.00 H 693 2HD1 LEU A 49152.169 6.408 -7.012 1.00 0.00 H ATOM 694 3HD1 LEU A 49152.530 6.540 -5.290 1.00 0.00 H **ATOM** ATOM 695 1HD2 LEU A 49149.181 4.891 -6.742 1.00 0.00 H ATOM 696 2HD2 LEU A 49150.438 4.149 -5.751 1.00 0.00 H 697 3HD2 LEU A 49150.854 4.882 -7.301 1.00 0.00 H ATOM 698 N ALAA 50147.943 5.072 -1.846 1.00 0.00 N ATOM 699 CA ALA A 50147.794 4.702 -0.446 1.00 0.00 C ATOM 700 C ALAA 50148.728 3.553 -0.081 1.00 0.00 C ATOM 701 O ALAA 50148.587 2.440 -0.588 1.00 0.00 O **ATOM** 702 CB ALAA 50146.350 4.325 -0.152 1.00 0.00 C ATOM ATOM 703 H ALA A 50147.405 4.613 -2.524 1.00 0.00 H 704 HA ALA A 50148.047 5.565 0.151 1.00 0.00 H ATOM 705 1HB ALA A 50145.908 3.878 -1.029 1.00 0.00 H **ATOM** 706 2HB ALA A 50145.795 5.211 0.119 1.00 0.00 H ATOM ATOM - 707 3HB ALA A 50146.321 3.620 0.666 1.00 0.00 H 708 N GLY A 51149.682 3.830 0.801 1.00 0.00 N ATOM 709 CA GLY A 51150.625 2.809 1.219 1.00 0.00 C **ATOM** 710 C GLYA 51149.976 1.735 2.070 1.00 0.00 C ATOM 711 O GLY A 51149.657 1.965 3.236 1.00 0.00 O **ATOM** 712 H GLY A 51149.746 4.734 1.173 1.00 0.00 H **ATOM** 713 1HA GLY A 51151.052 2.348 0.341 1.00 0.00 H **ATOM** 714 2HA GLY A 51151.414 3.275 1.789 1.00 0.00 H **ATOM** 715 N LEUA 52149.779 0.557 1.485 1.00 0.00 N ATOM **ATOM** 716 CA LEU A 52149.164 -0.556 2.198 1.00 0.00 C 717 C LEUA 52150.224 -1.465 2.808 1.00 0.00 C

718 O LEUA 52151.150 -1.902 2.125 1.00 0.00 O **ATOM** 719 CB LEU A 52148.265 -1.358 1.256 1.00 0.00 C **ATOM** 720 CG LEUA 52147.001 -0.634 0.792 1.00 0.00 C ATOM **ATOM** 721 CD1 LEU A 52146.360 -1.372 -0.373 1.00 0.00 C 722 CD2 LEU A 52146.016 -0.493 1.943 1.00 0.00 C **ATOM** 723 H LEUA 52150.054 0.434 0.553 1.00 0.00 H ATOM 724 HA LEU A 52148.559 -0.145 2.994 1.00 0.00 H ATOM 725 1HB LEU A 52148.844 -1.626 0.383 1.00 0.00 H **ATOM** 726 2HB LEUA 52147.968 -2.266 1.761 1.00 0.00 H ATOM 727 HG LEU A 52147.265 0.358 0.453 1.00 0.00 H **ATOM** 728 1HD1 LEU A 52146.068 -2.362 -0.055 1.00 0.00 H **ATOM** 729 2HD1 LEU A 52147.069 -1.448 -1.184 1.00 0.00 H ATOM **ATOM** 730 3HD1 LEU A 52145.488 -0.829 -0.707 1.00 0.00 H 731 1HD2 LEU A 52145.198 0.145 1.641 1.00 0.00 H ATOM 732 2HD2 LEU A 52146.517 -0.057 2.794 1.00 0.00 H ATOM 733 3HD2 LEU A 52145.633 -1.467 2.211 1.00 0.00 H ATOM 734 N GLUA 53150.082 -1.748 4.100 1.00 0.00 N ATOM 735 CA GLUA 53151.027 -2.607 4.802 1.00 0.00 C ATOM 736 C GLUA 53150.520 -4.044 4.856 1.00 0.00 C **ATOM** 737 O GLUA 53149.535 -4.340 5.532 1.00 0.00 O ATOM 738 CB GLUA 53151.266 -2.085 6.221 1.00 0.00 C **ATOM** 739 CG GLUA 53152.268 -2.908 7.013 1.00 0.00 C ATOM 740 CD GLUA 53151.835 -3.131 8.448 1.00 0.00 C **ATOM** 741 OE1 GLUA 53151.291 -4.216 8.744 1.00 0.00 O **ATOM** 742 OE2 GLU A 53152.041 -2.220 9.279 1.00 0.00 O **ATOM** 743 H GLUA 53149.323 -1.370 4.591 1.00 0.00 H **ATOM** 744 HA GLUA 53151.961 -2.587 4.259 1.00 0.00 H ATOM 745 1HB GLU A 53151.633 -1.071 6.162 1.00 0.00 H ATOM 746 2HB GLU A 53150.327 -2.087 6.756 1.00 0.00 H **ATOM** 747 1HG GLUA 53152.382 -3.870 6.534 1.00 0.00 H ATOM 748 2HG GLU A 53153.217 -2.393 7.013 1.00 0.00 H ATOM

749 N LEUA 54151.200 -4.933 4.139 1.00 0.00 N 750 CA LEUA 54150.817 -6.340 4.105 1.00 0.00 C ATOM 751 C LEUA 54151.111 -7.016 5.440 1.00 0.00 C **ATOM** 752 O LEUA 54152.156 -6.782 6.049 1.00 0.00 O ATOM ATOM 753 CB LEU A 54151.558 -7.064 2.979 1.00 0.00 C ATOM 754 CG LEUA 54151.517 -6.362 1.621 1.00 0.00 C 755 CD1 LEU A 54152.750 -6.710 0.802 1.00 0.00 C **ATOM** 756 CD2 LEU A 54150.250 -6.737 0.867 1.00 0.00 C **ATOM** 757 H LEUA 54151.976 -4.637 3.621 1.00 0.00 H **ATOM ATOM** 758 HA LEU A 54149.755 -6.390 3.916 1.00 0.00 H ATOM 759 1HB LEU A 54152.592 -7.178 3.272 1.00 0.00 H 760 2HB LEU A 54151.123 -8.046 2.864 1.00 0.00 H **ATOM** 761 HG LEUA 54151.510 -5.293 1.776 1.00 0.00 H ATOM 762 1HD1 LEU A 54152.593 -6.419 -0.226 1.00 0.00 H **ATOM ATOM** 763 2HD1 LEU A 54152.926 -7.775 0.853 1.00 0.00 H 764 3HD1 LEU A 54153.605 -6.184 1.199 1.00 0.00 H ATOM ATOM 765 1HD2 LEU A 54150.238 -7.803 0.691 1.00 0.00 H 766 2HD2 LEU A 54150.227 -6.216 -0.080 1.00 0.00 H ATOM **ATOM** 767 3HD2 LEU A 54149.386 -6.459 1.452 1.00 0.00 H ATOM 768 N GLUA 55150.185 -7.857 5.890 1.00 0.00 N 769 CA GLUA 55150.346 -8.568 7.153 1.00 0.00 C ATOM 770 C GLUA 55151.400 -9.662 7.031 1.00 0.00 C ATOM 771 O GLUA 55152.098 -9.977 7.995 1.00 0.00 O **ATOM** 772 CB GLUA 55149.013 -9.174 7.594 1.00 0.00 C ATOM 773 CG GLUA 55148.076 -8.172 8.249 1.00 0.00 C **ATOM** 774 CD GLUA 55146.632 -8.363 7.827 1.00 0.00 C ATOM 775 OE1 GLU A 55145.767 -8.503 8.717 1.00 0.00 O **ATOM ATOM** 776 OE2 GLU A 55146.366 -8.371 6.606 1.00 0.00 O 777 H GLUA 55149.374 -8.002 5.359 1.00 0.00 H ATOM **ATOM** 778 HA GLU A 55150.670 -7.853 7.895 1.00 0.00 H 779 1HB GLU A 55148.515 -9.588 6.730 1.00 0.00 H ATOM

780 2HB GLU A 55149.207 -9.967 8.301 1.00 0.00 H **ATOM** 781 1HG GLUA 55148.139 -8.286 9.321 1.00 0.00 H **ATOM** 782 2HG GLUA 55148.387 -7.174 7.974 1.00 0.00 H **ATOM** 783 N ASPA 56151.511 -10.239 5.839 1.00 0.00 N **ATOM** 784 CA ASP A 56152.481 -11.300 5.590 1.00 0.00 C ATOM **ATOM** 785 C ASPA 56153.770 -10.732 5.004 1.00 0.00 C 786 O ASPA 56153.744 -10.008 4.008 1.00 0.00 O ATOM **ATOM** 787 CB ASP A 56151.893 -12.345 4.642 1.00 0.00 C **ATOM** 788 CG ASP A 56151.185 -13.464 5.381 1.00 0.00 C 789 OD1 ASP A 56151.383 -14.640 5.009 1.00 0.00 O **ATOM** 790 OD2 ASP A 56150.434 -13.164 6.333 1.00 0.00 O **ATOM** 791 H ASPA 56150.927 -9.945 5.109 1.00 0.00 H ATOM 792 HA ASPA 56152.707 -11.770 6.535 1.00 0.00 H **ATOM** 793 1HB ASPA 56151.181 -11.867 3.985 1.00 0.00 H ATOM 794 2HB ASP A 56152.688 -12.775 4.051 1.00 0.00 H **ATOM** 795 N GLUA 57154.895 -11.065 5.626 1.00 0.00 N **ATOM** 796 CA GLUA 57156.194 -10.588 5.166 1.00 0.00 C **ATOM** 797 C GLUA 57156.577 -11.245 3.845 1.00 0.00 C ATOM 798 O GLUA 57157.029 -12.390 3.817 1.00 0.00 O ATOM 799 CB GLU A 57157.267 -10.870 6.220 1.00 0.00 C ATOM 800 CG GLU A 57157.447 -9.740 7.221 1.00 0.00 C **ATOM** 801 CD GLUA 57158.872 -9.634 7.728 1.00 0.00 C ATOM 802 OE1 GLU A 57159.805 -9.697 6.900 1.00 0.00 O ATOM 803 OE2 GLU A 57159.056 -9.488 8.955 1.00 0.00 O **ATOM** 804 H GLUA 57154.851 -11.645 6.416 1.00 0.00 H ATOM 805 HA GLU A 57156.121 -9.522 5.016 1.00 0.00 H **ATOM** 806 1HB GLU A 57156.996 -11.764 6.763 1.00 0.00 H **ATOM** 807 2HB GLUA 57158.211 -11.035 5.721 1.00 0.00 H **ATOM** ATOM. 808 1HG GLUA 57157.181 -8.809 6.746 1.00 0.00 H **ATOM** 809 2HG GLUA 57156.793 -9.914 8.062 1.00 0.00 H 810 N CYS A 58156.395 -10.513 2.750 1.00 0.00 N

- ATOM 811 CA CYS A 58156.722 -11.025 1.425 1.00 0.00 C
- ATOM 812 C CYS A 58158.004 -10.389 0.898 1.00 0.00 C
- ATOM 813 O CYS A 58158.094 -9.169 0.762 1.00 0.00 O
- ATOM 814 CB CYS A 58155.570 -10.760 0.454 1.00 0.00 C
- ATOM 815 SG CYS A 58154.347 -12.089 0.379 1.00 0.00 S
- ATOM 816 H CYS A 58156.032 -9.607 2.837 1.00 0.00 H
- ATOM 817 HA CYS A 58156.872 -12.091 1.509 1.00 0.00 H
- ATOM 818 1HB CYS A 58155.057 -9.858 0.754 1.00 0.00 H
- ATOM 819 2HB CYS A 58155.972 -10.625 -0.540 1.00 0.00 H
- ATOM 820 HG CYS A 58154.819 -12.920 0.284 1.00 0.00 H
- ATOM 821 N ALAA 59158.995 -11.225 0.602 1.00 0.00 N
- ATOM 822 CA ALA A 59160.272 -10.744 0.090 1.00 0.00 C
- ATOM 823 C ALAA 59160.092 -10.017 -1.238 1.00 0.00 C
- ATOM 824 O ALAA 59159.556 -10.575 -2.195 1.00 0.00 O
- ATOM 825 CB ALA A 59161.246 -11.902 -0.069 1.00 0.00 C
- ATOM 826 H ALAA 59158.864 -12.187 0.732 1.00 0.00 H
- ATOM 827 HA ALA A 59160.683 -10.055 0.813 1.00 0.00 H
- ATOM 828 1HB ALA A 59161.919 -11.697 -0.889 1.00 0.00 H
- ATOM 829 2HB ALA A 59160.697 -12.809 -0.272 1.00 0.00 H
- ATOM 830 3HB ALA A 59161.814 -12.021 0.841 1.00 0.00 H
- ATOM 831 N GLY A 60160.541 -8.767 -1.288 1.00 0.00 N
- ATOM 832 CA GLY A 60160.420 -7.984 -2.504 1.00 0.00 C
- ATOM 833 C GLY A 60159.945 -6.569 -2.237 1.00 0.00 C
- ATOM 834 O GLY A 60160.265 -5.647 -2.989 1.00 0.00 O
- ATOM 835 H GLY A 60160.959 -8.373 -0.494 1.00 0.00 H
- ATOM 836 1HA GLY A 60161.382 -7.943 -2.991 1.00 0.00 H
- ATOM 837 2HA GLY A 60159.715 -8.469 -3.163 1.00 0.00 H
- ATOM 838 N CYS A 61159.183 -6.395 -1.163 1.00 0.00 N
- ATOM 839 CA CYS A 61158.664 -5.082 -0.798 1.00 0.00 C
- ATOM 840 C CYS A 61159.626 -4.359 0.140 1.00 0.00 C
- ATOM 841 O CYS A 61160.633 -4.922 0.567 1.00 0.00 O

- ATOM 842 CB CYS A 61157.293 -5.218 -0.136 1.00 0.00 C
- ATOM 843 SG CYS A 61156.080 -6.119 -1.129 1.00 0.00 S
- ATOM 844 H CYS A 61158.963 -7.168 -0.602 1.00 0.00 H
- ATOM 845 HA CYS A 61158.561 -4.503 -1.704 1.00 0.00 H
- ATOM 846 1HB CYS A 61157.403 -5.742 0.801 1.00 0.00 H
- ATOM 847 2HB CYS A 61156.894 -4.232 0.055 1.00 0.00 H
- ATOM 848 HG CYS A 61156.127 -5.787 -2.029 1.00 0.00 H
- ATOM 849 N THR A 62159.306 -3.107 0.457 1.00 0.00 N
- ATOM 850 CA THR A 62160.142 -2.308 1.345 1.00 0.00 C
- ATOM 851 C THR A 62159.530 -2.225 2.739 1.00 0.00 C
- ATOM 852 O THR A 62158.568 -2.929 3.048 1.00 0.00 O
- ATOM 853 CB THR A 62160.329 -0.902 0.774 1.00 0.00 C
- ATOM 854 OG1 THR A 62159.146 -0.138 0.925 1.00 0.00 O
- ATOM 855 CG2 THR A 62160.696 -0.896 -0.695 1.00 0.00 C
- ATOM 856 H THR A 62158.490 -2.714 0.084 1.00 0.00 H
- ATOM 857 HA THR A 62161.106 -2.789 1.416 1.00 0.00 H
- ATOM 858 HB THR A 62161.123 -0.407 1.314 1.00 0.00 H
- ATOM 859 HG1 THR A 62158.400 -0.629 0.572 1.00 0.00 H
- ATOM 860 1HG2 THR A 62161.182 0.036 -0.941 1.00 0.00 H
- ATOM 861 2HG2 THR A 62159.800 -1.003 -1.290 1.00 0.00 H
- ATOM 862 3HG2 THR A 62161.365 -1.718 -0.902 1.00 0.00 H
- ATOM 863 N ASPA 63160.095 -1.362 3.578 1.00 0.00 N
- ATOM 864 CA ASPA 63159.605 -1.188 4.940 1.00 0.00 C
- ATOM 865 C ASPA 63158.822 0.115 5.073 1.00 0.00 C
- ATOM 866 O ASPA 63158.815 0.740 6.134 1.00 0.00 O
- ATOM 867 CB ASP A 63160.772 -1.199 5.930 1.00 0.00 C
- ATOM 868 CG ASP A 63161.778 -0.100 5.649 1.00 0.00 C
- ATOM 869 OD1 ASP A 63162.909 -0.422 5.230 1.00 0.00 O
- ATOM 870 OD2 ASP A 63161.434 1.085 5.850 1.00 0.00 O
- ATOM 871 H ASPA 63160.860 -0.830 3.272 1.00 0.00 H
- ATOM 872 HA ASP A 63158.947 -2.013 5.164 1.00 0.00 H

873 1HB ASPA 63160.389 -1.064 6.930 1.00 0.00 H ATOM ATOM 874 2HB ASPA 63161.279 -2.151 5.867 1.00 0.00 H **ATOM** 875 N GLY A 64158.166 0.519 3.991 1.00 0.00 N 876 CA GLY A 64157.389 1.744 4.009 1.00 0.00 C ATOM 877 C GLY A 64158.114 2.900 3.347 1.00 0.00 C ATOM ATOM 878 O GLYA 64158.167 4.002 3.892 1.00 0.00 O **ATOM** 879 H GLY A 64158.208 -0.020 3.174 1.00 0.00 H 880 1HA GLY A 64156.457 1.574 3.492 1.00 0.00 H **ATOM** 881 2HA GLY A 64157.177 2.008 5.035 1.00 0.00 H **ATOM ATOM** 882 N THR A 65158.674 2.647 2.168 1.00 0.00 N **ATOM** 883 CA THR A 65159.399 3.675 1.431 1.00 0.00 C **ATOM** 884 C THR A 65159.023 3.652 -0.047 1.00 0.00 C 885 O THR A 65159.172 2.632 -0.720 1.00 0.00 O ATOM 886 CB THR A 65160.908 3.476 1.589 1.00 0.00 C **ATOM** 887 OG1 THR A 65161.327 2.287 0.941 1.00 0.00 O ATOM 888 CG2 THR A 65161.353 3.394 3.032 1.00 0.00 C **ATOM** 889 H THR A 65158.598 1.748 1.786 1.00 0.00 H ATOM 890 HA THR A 65159.127 4.635 1.845 1.00 0.00 H **ATOM** 891 HB THR A 65161.420 4.310 1.131 1.00 0.00 H ATOM **ATOM** 892 HG1 THR A 65160.733 1.570 1.174 1.00 0.00 H **ATOM** 893 1HG2 THR A 65161.703 2.395 3.245 1.00 0.00 H **ATOM** 894 2HG2 THR A 65160.521 3.631 3.680 1.00 0.00 H **ATOM** 895 3HG2 THR A 65162.154 4.099 3.203 1.00 0.00 H 896 N PHE A 66158.536 4.784 -0.546 1.00 0.00 N **ATOM** 897 CA PHE A 66158.138 4.894 -1.945 1.00 0.00 C **ATOM** 898 C PHE A 66159.106 5.785 -2.717 1.00 0.00 C **ATOM ATOM** 899 O PHE A 66159.243 6.971 -2.422 1.00 0.00 O 900 CB PHEA 66156.718 5.452 -2.051 1.00 0.00 C **ATOM** 901 CG PHE A 66156.051 5.152 -3.362 1.00 0.00 C **ATOM** 902 CD1 PHE A 66155.567 6.177 -4.159 1.00 0.00 C **ATOM** 903 CD2 PHE A 66155.908 3.844 -3.798 1.00 0.00 C **ATOM**

904 CE1 PHE A 66154.953 5.903 -5.367 1.00 0.00 C ATOM 905 CE2 PHE A 66155.294 3.564 -5.004 1.00 0.00 C **ATOM ATOM** 906 CZ PHE A 66154.816 4.596 -5.790 1.00 0.00 C 907 H PHE A 66158.441 5.563 0.040 1.00 0.00 H ATOM 908 HA PHE A 66158.159 3.904 -2.374 1.00 0.00 H **ATOM** 909 1HB PHE A 66156.112 5.028 -1.265 1.00 0.00 H ATOM: **ATOM** 910 2HB PHE A 66156.752 6.526 -1.931 1.00 0.00 H 911 HD1 PHE A 66155.674 7.200 -3.829 1.00 0.00 H **ATOM** 912 HD2 PHE A 66156.282 3.037 -3.185 1.00 0.00 H **ATOM** 913 HE1 PHE A 66154.579 6.711 -5.978 1.00 0.00 H **ATOM** 914 HE2 PHE A 66155.189 2.541 -5.333 1.00 0.00 H ATOM **ATOM** 915 HZ PHE A 66154.337 4.379 -6.732 1.00 0.00 H 916 N ARGA 67159.776 5.204 -3.706 1.00 0.00 N ATOM 917 CA ARG A 67160.732 5.945 -4.521 1.00 0.00 C ATOM 918 C ARG A 67161.860 6.505 -3.662 1.00 0.00 C **ATOM** 919 O ARG A 67162.359 7.602 -3.913 1.00 0.00 O ATOM 920 CB ARG A 67160.026 7.082 -5.263 1.00 0.00 C ATOM **ATOM** 921 CG ARG A 67158.955 6.606 -6.229 1.00 0.00 C 922 CD ARG A 67158.909 7.468 -7.481 1.00 0.00 C ATOM 923 NE ARG A 67160.062 7.236 -8.347 1.00 0.00 N **ATOM** 924 CZ ARG A 67160.434 8.061 -9.323 1.00 0.00 C **ATOM** 925 NH1 ARG A 67159.746 9.171 -9.562 1.00 0.00 N **ATOM** 926 NH2 ARG A 67161.496 7.775 -10.064 1.00 0.00 N ATOM **ATOM** 927 H ARG A 67159.624 4.254 -3.893 1.00 0.00 H 928 HA ARG A 67161.150 5.261 -5.244 1.00 0.00 H ATOM 929 1HB ARG A 67159.564 7.736 -4.539 1.00 0.00 H ATOM 930 2HB ARG A 67160.762 7.642 -5.822 1.00 0.00 H **ATOM** 931 1HG ARG A 67159.166 5.587 -6.514 1.00 0.00 H ATOM ATOM 932 2HG ARG A 67157.994 6.651 -5.736 1.00 0.00 H 933 1HD ARG A 67158.008 7.237 -8.029 1.00 0.00 H ATOM ATOM 934 2HD ARG A 67158.894 8.507 -7.186 1.00 0.00 H

- ATOM 935 HE ARG A 67160.588 6.424 -8.193 1.00 0.00 H
- ATOM 936 1HH1 ARG A 67158.944 9.393 -9.007 1.00 0.00 H
- ATOM 937 2HH1 ARG A 67160.030 9.786 -10.297 1.00 0.00 H
- ATOM 938 1HH2 ARG A 67162.018 6.940 -9.888 1.00 0.00 H
- ATOM 939 2HH2 ARG A 67161.775 8.395 -10.798 1.00 0.00 H
- ATOM 940 N GLY A 68162.258 5.744 -2.648 1.00 0.00 N
- ATOM 941 CA GLY A 68163.326 6.180 -1.767 1.00 0.00 C
- ATOM 942 C GLY A 68162.888 7.290 -0.831 1.00 0.00 C
- ATOM 943 O GLY A 68163.699 8.118 -0.417 1.00 0.00 O
- ATOM 944 H GLY A 68161.824 4.879 -2.497 1.00 0.00 H
- ATOM 945 1HA GLY A 68163.660 5.339 -1.179 1.00 0.00 H
- ATOM 946 2HA GLY A 68164.150 6.537 -2.368 1.00 0.00 H
- ATOM 947 N THR A 69161.602 7.306 -0.497 1.00 0.00 N
- ATOM 948 CA THR A 69161.057 8.321 0.396 1.00 0.00 C
- ATOM 949 C THR A 69160.168 7.689 1.461 1.00 0.00 C
- ATOM 950 O THR A 69159.055 7.247 1.174 1.00 0.00 O
- ATOM 951 CB THR A 69160.261 9.357 -0.401 1.00 0.00 C
- ATOM 952 OG1 THR A 69160.900 9.644 -1.631 1.00 0.00 O
- ATOM 953 CG2 THR A 69160.075 10.666 0.336 1.00 0.00 C
- ATOM 954 H THR A 69161.005 6.618 -0.860 1.00 0.00 H
- ATOM 955 HA THR A 69161.886 8.814 0.882 1.00 0.00 H
- ATOM 956 HB THR A 69159.281 8.955 -0.614 1.00 0.00 H
- ATOM 957 HG1 THR A 69161.773 10.008 -1.461 1.00 0.00 H
- ATOM 958 1HG2 THR A 69160.256 11.488 -0.340 1.00 0.00 H
- ATOM 959 2HG2 THR A 69160.772 10.717 1.160 1.00 0.00 H
- ATOM 960 3HG2 THR A 69159.065 10.725 0.714 1.00 0.00 H
- ATOM 961 N ARG A 70160.666 7.649 2.693 1.00 0.00 N
- ATOM 962 CA ARG A 70159.916 7.070 3.801 1.00 0.00 C
- ATOM 963 C ARG A 70158.751 7.971 4.200 1.00 0.00 C
- ATOM 964 O ARG A 70158.945 9.137 4.541 1.00 0.00 O
- ATOM 965 CB ARG A 70160.835 6.844 5.004 1.00 0.00 C

ATOM 966 CG ARG A 70160.136 6.206 6.193 1.00 0.00 C 967 CD ARG A 70160.931 6.397 7.474 1.00 0.00 C **ATOM** ATOM 968 NE ARG A 70162.034 5.445 7.582 1.00 0.00 N **ATOM** 969 CZ ARG A 70163.054 5.585 8.426 1.00 0.00 C **ATOM** 970 NH1 ARG A 70163.116 6.635 9.235 1.00 0.00 N **ATOM** 971 NH2 ARG A 70164.015 4.673 8.459 1.00 0.00 N **ATOM** 972 H ARG A 70161.559 8.016 2.860 1.00 0.00 H **ATOM** 973 HA ARG A 70159.524 6.118 3.476 1.00 0.00 H **ATOM** 974 1HB ARG A 70161.649 6.200 4.704 1.00 0.00 H 975 2HB ARG A 70161.239 7.796 5.318 1.00 0.00 H ATOM **ATOM** 976 1HG ARG A 70159.164 6.660 6.312 1.00 0.00 H 977 2HG ARG A 70160.020 5.149 6.005 1.00 0.00 H ATOM ATOM 978 1HD ARG A 70161.331 7.400 7.489 1.00 0.00 H 979 2HD ARG A 70160.268 6.263 8.317 1.00 0.00 H ATOM 980 HE ARG A 70162.013 4.661 6.995 1.00 0.00 H ATOM ATOM 981 1HH1 ARG A 70162.394 7.327 9.215 1.00 0.00 H 982 2HH1 ARG A 70163.885 6.734 9.866 1.00 0.00 H ATOM ATOM 983 1HH2 ARG A 70163.974 3.880 7.851 1.00 0.00 H **ATOM** 984 2HH2 ARG A 70164.782 4.778 9.092 1.00 0.00 H **ATOM** 985 N TYR A 71157.543 7.421 4.154 1.00 0.00 N 986 CA TYR A 71156.346 8.176 4.510 1.00 0.00 C ATOM **ATOM** 987 C TYR A 71155.852 7.788 5.900 1.00 0.00 C 988 O TYR A 71155.446 8.644 6.686 1.00 0.00 O ATOM 989 CB TYR A 71155.242 7.936 3.479 1.00 0.00 C **ATOM** 990 CG TYR A 71155.536 8.538 2.124 1.00 0.00 C ATOM 991 CD1 TYR A 71156.048 9.825 2.011 1.00 0.00 C ATOM 992 CD2 TYR A 71155.304 7.820 0.958 1.00 0.00 C ATOM 993 CE1 TYR A 71156.318 10.379 0.773 1.00 0.00 C **ATOM** 994 CE2 TYR A 71155.572 8.367 -0.283 1.00 0.00 C ATOM ATOM 995 CZ TYR A 71156.079 9.647 -0.369 1.00 0.00 C 996 OH TYR A 71156.347 10.193 -1.603 1.00 0.00 O ATOM

997 H TYR A 71157.452 6.487 3.874 1.00 0.00 H **ATOM** 998 HA TYR A 71156.604 9.224 4.511 1.00 0.00 H ATOM ATOM 999 1HB TYR A 71155.106 6.873 3.346 1.00 0.00 H ATOM 1000 2HB TYR A 71154.321 8.368 3.842 1.00 0.00 H ATOM 1001 HD1 TYR A 71156.234 10.397 2.908 1.00 0.00 H ATOM 1002 HD2 TYR A 71154.906 6.819 1.029 1.00 0.00 H ATOM 1003 HE1 TYR A 71156.716 11.381 0.706 1.00 0.00 H ATOM 1004 HE2 TYR A 71155.384 7.793 -1.178 1.00 0.00 H ATOM 1005 HH TYR A 71157.236 9.952 -1.874 1.00 0.00 H ATOM 1006 N PHE A 72155.891 6.494 6.197 1.00 0.00 N ATOM 1007 CA PHE A 72155.448 5.993 7.492 1.00 0.00 C ATOM 1008 C PHE A 72156.433 4.968 8.045 1.00 0.00 C ATOM 1009 O PHE A 72157.368 4.556 7.358 1.00 0.00 O ATOM 1010 CB PHE A 72154.057 5.368 7.373 1.00 0.00 C ATOM 1011 CG PHE A 72153.981 4.262 6.359 1.00 0.00 C ATOM 1012 CD1 PHE A 72154.205 2.946 6.733 1.00 0.00 C ATOM 1013 CD2 PHE A 72153.686 4.538 5.034 1.00 0.00 C ATOM 1014 CE1 PHE A 72154.135 1.926 5.802 1.00 0.00 C ATOM 1015 CE2 PHE A 72153.616 3.522 4.099 1.00 0.00 C ATOM 1016 CZ PHE A 72153.841 2.214 4.484 1.00 0.00 C ATOM 1017 H PHE A 72156.226 5.859 5.528 1.00 0.00 H ATOM 1018 HA PHE A 72155.399 6.831 8.172 1.00 0.00 H ATOM 1019 1HB PHE A 72153.769 4.961 8.330 1.00 0.00 H ATOM 1020 2HB PHE A 72153.350 6.133 7.084 1.00 0.00 H ATOM 1021 HD1 PHE A 72154.434 2.719 7.763 1.00 0.00 H ATOM 1022 HD2 PHE A 72153.511 5.560 4.731 1.00 0.00 H ATOM 1023 HE1 PHE A 72154.311 0.905 6.106 1.00 0.00 H ATOM 1024 HE2 PHE A 72153.386 3.751 3.069 1.00 0.00 H ATOM 1025 HZ PHE A 72153.786 1.419 3.756 1.00 0.00 H ATOM 1026 N THR A 73156.216 4.559 9.291 1.00 0.00 N ATOM 1027 CA THR A 73157.085 3.581 9.937 1.00 0.00 C

ATOM 1028 C THR A 73156.374 2.242 10.094 1.00 0.00 C ATOM 1029 O THR A 73155.396 2.129 10.834 1.00 0.00 O ATOM 1030 CB THR A 73157.538 4.094 11.304 1.00 0.00 C ATOM 1031 OG1 THR A 73157.838 5.477 11.247 1.00 0.00 O ATOM 1032 CG2 THR A 73158.761 3.380 11.837 1.00 0.00 C ATOM 1033 H THR A 73155.455 4.923 9.789 1.00 0.00 H ATOM 1034 HA THR A 73157.952 3.443 9.309 1.00 0.00 H ATOM 1035 HB THR A 73156.736 3.951 12.015 1.00 0.00 H ATOM 1036 HG1 THR A 73157.472 5.918 12.018 1.00 0.00 H ATOM 1037 1HG2 THR A 73159.373 4.077 12.389 1.00 0.00 H ATOM 1038 2HG2 THR A 73159.331 2.978 11.011 1.00 0.00 H ATOM 1039 3HG2 THR A 73158.454 2.575 12.487 1.00 0.00 H ATOM 1040 N CYS A 74156.871 1.227 9.394 1.00 0.00 N ATOM 1041 CA CYS A 74156.282 -0.106 9.455 1.00 0.00 C ATOM 1042 C CYS A 74157.366 -1.179 9.459 1.00 0.00 C ATOM 1043 O CYS A 74158.558 -0.871 9.475 1.00 0.00 O ATOM 1044 CB CYS A 74155.336 -0.324 8.272 1.00 0.00 C ATOM 1045 SG CYS A 74153.626 0.165 8.594 1.00 0.00 S ATOM 1046 H CYS A 74157.652 1.380 8.821 1.00 0.00 H ATOM 1047 HA CYS A 74155.718 -0.177 10.373 1.00 0.00 H ATOM 1048 1HB CYS A 74155.688 0.251 7.429 1.00 0.00 H ATOM 1049 2HB CYS A 74155.336 -1.372 8.011 1.00 0.00 H ATOM 1050 HG CYS A 74153.519 0.260 9.543 1.00 0.00 H ATOM 1051 N ALA A 75156.944 -2.438 9.446 1.00 0.00 N ATOM 1052 CA ALA A 75157.878 -3.557 9.448 1.00 0.00 C ATOM 1053 C ALAA 75158.504 -3.753 8.071 1.00 0.00 C ATOM 1054 O ALAA 75158.021 -3.212 7.077 1.00 0.00 O ATOM 1055 CB ALA A 75157.177 -4.830 9.897 1.00 0.00 C ATOM 1056 H ALA A 75155.981 -2.620 9.434 1.00 0.00 H ATOM 1057 HA ALA A 75158.661 -3.336 10.159 1.00 0.00 H ATOM 1058 1HB ALA A 75156.438 -4.588 10.647 1.00 0.00 H

ATOM 1059 2HB ALA A 75157.902 -5.513 10.314 1.00 0.00 H ATOM 1060 3HB ALA A 75156.692 -5.292 9.049 1.00 0.00 H ATOM 1061 N LEUA 76159.581 -4.530 8.021 1.00 0.00 N ATOM 1062 CA LEU A 76160.273 -4.798 6.765 1.00 0.00 C ATOM 1063 C LEUA 76159.514 -5.828 5.935 1.00 0.00 C ATOM 1064 O LEUA 76158.956 -6.784 6.473 1.00 0.00 O ATOM 1065 CB LEU A 76161.695 -5.292 7.037 1.00 0.00 C ATOM 1066 CG LEU A 76162.712 -4.195 7.352 1.00 0.00 C ATOM 1067 CD1 LEU A 76163.770 -4.708 8.317 1.00 0.00 C ATOM 1068 CD2 LEU A 76163.358 -3.686 6.072 1.00 0.00 C ATOM 1069 H LEUA 76159.919 -4.933 8.848 1.00 0.00 H ATOM 1070 HA LEU A 76160.323 -3.872 6.212 1.00 0.00 H ATOM 1071 1HB LEU A 76161.661 -5.975 7.874 1.00 0.00 H ATOM 1072 2HB LEU A 76162.038 -5.832 6.168 1.00 0.00 H ATOM 1073 HG LEU A 76162.204 -3.366 7.824 1.00 0.00 H ATOM 1074 1HD1 LEU A 76164.717 -4.240 8.096 1.00 0.00 H ATOM 1075 2HD1 LEU A 76163.865 -5.779 8.210 1.00 0.00 H ATOM 1076 3HD1 LEU A 76163.478 -4.472 9.330 1.00 0.00 H ATOM 1077 1HD2 LEU A 76162.688 -3.851 5.241 1.00 0.00 H ATOM 1078 2HD2 LEU A 76164.282 -4.216 5.899 1.00 0.00 H ATOM 1079 3HD2 LEU A 76163.562 -2.630 6.166 1.00 0.00 H ATOM 1080 N LYS A 77159.498 -5.627 4.621 1.00 0.00 N ATOM 1081 CA LYS A 77158.807 -6.538 3.716 1.00 0.00 C ATOM 1082 C LYS A 77157.311 -6.563 4.005 1.00 0.00 C ATOM 1083 O LYS A 77156.676 -7.618 3.962 1.00 0.00 O ATOM 1084 CB LYS A 77159.387 -7.948 3.836 1.00 0.00 C ATOM 1085 CG LYS A 77160.907 -7.984 3.832 1.00 0.00 C ATOM 1086 CD LYS A 77161.469 -7.583 2.478 1.00 0.00 C ATOM 1087 CE LYS A 77162.944 -7.228 2.570 1.00 0.00 C ATOM 1088 NZ LYS A 77163.150 -5.792 2.908 1.00 0.00 N ATOM 1089 H LYS A 77159.962 -4.846 4.252 1.00 0.00 H

ATOM 1090 HA LYS A 77158.960 -6.181 2.707 1.00 0.00 H ATOM 1091 1HB LYS A 77159.041 -8.389 4.760 1.00 0.00 H ATOM 1092 2HB LYS A 77159.033 -8.544 3.008 1.00 0.00 H ATOM 1093 1HG LYS A 77161.275 -7.299 4.580 1.00 0.00 H ATOM 1094 2HG LYS A 77161.235 -8.987 4.066 1.00 0.00 H ATOM 1095 1HD LYS A 77161.351 -8.408 1.791 1.00 0.00 H ATOM 1096 2HD LYS A 77160.924 -6.726 2.112 1.00 0.00 H ATOM 1097 1HE LYS A 77163,401 -7.837 3,337 1.00 0.00 H ATOM 1098 2HE LYS A 77163.412 -7.436 1.619 1.00 0.00 H ATOM 1099 1HZ LYS A 77163.311 -5.241 2.041 1.00 0.00 H ATOM 1100 2HZ LYS A 77163.976 -5.686 3.531 1.00 0.00 H ATOM 1101 3HZ LYS A 77162.312 -5.416 3.395 1.00 0.00 H ATOM 1102 N LYS A 78156.750 -5.395 4.301 1.00 0.00 N ATOM 1103 CA LYS A 78155.326 -5.284 4.597 1.00 0.00 C ATOM 1104 C LYS A 78154.793 -3.911 4.198 1.00 0.00 C ATOM 1105 O LYS A 78153.981 -3.318 4.908 1.00 0.00 O ATOM 1106 CB LYS A 78155.074 -5.529 6.086 1.00 0.00 C ATOM 1107 CG LYS A 78155.640 -6.847 6.590 1.00 0.00 C ATOM 1108 CD LYS A 78155.270 -7.094 8.043 1.00 0.00 C ATOM 1109 CE LYS A 78154.151 -8.116 8.169 1.00 0.00 C ATOM 1110 NZ LYS A 78153.312 -7.875 9.376 1.00 0.00 N ATOM 1111 H LYS A 78157.306 -4.589 4.318 1.00 0.00 H ATOM 1112 HA LYS A 78154.809 -6.038 4.024 1.00 0.00 H ATOM 1113 1HB LYS A 78155.525 -4.728 6.653 1.00 0.00 H ATOM 1114 2HB LYS A 78154.009 -5.529 6.264 1.00 0.00 H ATOM 1115 1HG LYS A 78155.244 -7.651 5.986 1.00 0.00 H ATOM 1116 2HG LYS A 78156.716 -6.823 6.500 1.00 0.00 H ATOM 1117 1HD LYS A 78156.139 -7.463 8.568 1.00 0.00 H ATOM 1118 2HD LYS A 78154.947 -6.164 8.487 1.00 0.00 H ATOM 1119 1HE LYS A 78153.526 -8.055 7.291 1.00 0.00 H ATOM 1120 2HE LYS A 78154.586 -9.102 8.234 1.00 0.00 H

ATOM 1121 1HZ LYS A 78153.289 -6.859 9.599 1.00 0.00 H ATOM 1122 2HZ LYS A 78153.703 -8.388 10.191 1.00 0.00 H ATOM 1123 3HZ LYS A 78152.341 -8.205 9.207 1.00 0.00 H ATOM 1124 N ALA A 79155.255 -3.413 3.056 1.00 0.00 N ATOM 1125 CA ALA A 79154.824 -2.111 2.561 1.00 0.00 C ATOM 1126 C ALA A 79154.652 -2.129 1.047 1.00 0.00 C ATOM 1127 O ALAA 79155.630 -2.201 0.301 1.00 0.00 O ATOM 1128 CB ALAA 79155.822 -1.036 2.968 1.00 0.00 C ATOM 1129 H ALA A 79155.901 -3.932 2.534 1.00 0.00 H ATOM 1130 HA ALAA 79153.874 -1.878 3.019 1.00 0.00 H ATOM 1131 1HB ALAA 79155.857 -0.270 2.207 1.00 0.00 H ATOM 1132 2HB ALA A 79156.801 -1.477 3.080 1.00 0.00 H ATOM 1133 3HB ALA A 79155.515 -0.597 3.906 1.00 0.00 H ATOM 1134 N LEU A 80153.404 -2.063 0.597 1.00 0.00 N ATOM 1135 CA LEU A 80153.103 -2.072 -0.829 1.00 0.00 C ATOM 1136 C LEU A 80152.276 -0.851 -1.218 1.00 0.00 C ATOM 1137 O LEUA 80151.095 -0.756 -0.884 1.00 0.00 O ATOM 1138 CB LEU A 80152.352 -3.352 -1.205 1.00 0.00 C ATOM 1139 CG LEU A 80151.922 -3.444 -2.670 1.00 0.00 C ATOM 1140 CD1 LEU A 80153.135 -3.587 -3.575 1.00 0.00 C ATOM 1141 CD2 LEU A 80150.964 -4.609 -2.871 1.00 0.00 C ATOM 1142 H LEUA 80152.667 -2.007 1.240 1.00 0.00 H ATOM 1143 HA LEU A 80154.039 -2.044 -1.367 1.00 0.00 H ATOM 1144 1HB LEU A 80152.990 -4.195 -0.985 1.00 0.00 H ATOM 1145 2HB LEU A 80151.468 -3.420 -0.589 1.00 0.00 H ATOM 1146 HG LEUA 80151.406 -2.535 -2.944 1.00 0.00 H ATOM 1147 1HD1 LEU A 80152.858 -4.131 -4.466 1.00 0.00 H ATOM 1148 2HD1 LEU A 80153.913 -4.124 -3.052 1.00 0.00 H ATOM 1149 3HD1 LEU A 80153.497 -2.607 -3.850 1.00 0.00 H ATOM 1150 1HD2 LEU A 80151.527 -5.499 -3.113 1.00 0.00 H ATOM 1151 2HD2 LEU A 80150.285 -4.382 -3.679 1.00 0.00 H

ATOM 1152 3HD2 LEU A 80150.403 -4.774 -1.963 1.00 0.00 H ATOM 1153 N PHE A 81152.905 0.081 -1.927 1.00 0.00 N ATOM 1154 CA PHE A 81152.227 1.297 -2.362 1.00 0.00 C ATOM 1155 C PHE A 81151.405 1.041 -3.622 1.00 0.00 C ATOM 1156 O PHE A 81151.884 0.420 -4.571 1.00 0.00 O ATOM 1157 CB PHE A 81153.246 2.408 -2.621 1.00 0.00 C ATOM 1158 CG PHE A 81153.856 2.967 -1.367 1.00 0.00 C ATOM 1159 CD1 PHE A 81153,201 3,948 -0.640 1.00 0.00 C ATOM 1160 CD2 PHE A 81155.084 2.511 -0.916 1.00 0.00 C ATOM 1161 CE1 PHE A 81153.759 4.463 0.514 1.00 0.00 C ATOM 1162 CE2 PHE A 81155.649 3.023 0.237 1.00 0.00 C ATOM 1163 CZ PHE A 81154.985 4.000 0.953 1.00 0.00 C ATOM 1164 H PHE A 81153.846 -0.052 -2.164 1.00 0.00 H ATOM 1165 HA PHE A 81151.563 1.607 -1.570 1.00 0.00 H ATOM 1166 1HB PHE A 81154.045 2.019 -3.234 1.00 0.00 H ATOM 1167 2HB PHE A 81152.759 3.218 -3.145 1.00 0.00 H ATOM 1168 HD1 PHE A 81152.243 4.310 -0.982 1.00 0.00 H ATOM 1169 HD2 PHE A 81155.604 1.747 -1.476 1.00 0.00 H ATOM 1170 HE1 PHE A 81153.240 5.228 1.072 1.00 0.00 H ATOM 1171 HE2 PHE A 81156.607 2.659 0.578 1.00 0.00 H ATOM 1172 HZ PHE A 81155.424 4.401 1.854 1.00 0.00 H ATOM 1173 N VALA 82150.167 1.524 -3.623 1.00 0.00 N ATOM 1174 CA VAL A 82149.280 1.347 -4.765 1.00 0.00 C ATOM 1175 C VALA 82148.315 2.521 -4.898 1.00 0.00 C ATOM 1176 O VALA 82148.180 3.332 -3.983 1.00 0.00 O ATOM 1177 CB VALA 82148.470 0.042 -4.652 1.00 0.00 C ATOM 1178 CG1 VAL A 82149.379 -1.166 -4.809 1.00 0.00 C ATOM 1179 CG2 VAL A 82147.724 -0.010 -3.327 1.00 0.00 C ATOM 1180 H VALA 82149.843 2.010 -2.836 1.00 0.00 H ATOM 1181 HA VALA 82149.889 1.292 -5.656 1.00 0.00 H ATOM 1182 HB VALA 82147.742 0.022 -5.450 1.00 0.00 H

ATOM 1183 1HG1 VAL A 82150.018 -1.028 -5.668 1.00 0.00 H ATOM 1184 2HG1 VAL A 82148.779 -2.054 -4.947 1.00 0.00 H ATOM 1185 3HG1 VAL A 82149.987 -1.278 -3.923 1.00 0.00 H ATOM 1186 1HG2 VAL A 82147.242 -0.971 -3.223 1.00 0.00 H ATOM 1187 2HG2 VAL A 82146.979 0.771 -3.303 1.00 0.00 H ATOM 1188 3HG2 VAL A 82148.422 0.131 -2.515 1.00 0.00 H ATOM 1189 N LYS A 83147.645 2.602 -6.043 1.00 0.00 N ATOM 1190 CA LYS A 83146.693 3.677 -6.295 1.00 0.00 C ATOM 1191 C LYS A 83145.494 3.573 -5.358 1.00 0.00 C ATOM 1192 O LYS A 83144.809 2.552 -5.318 1.00 0.00 O ATOM 1193 CB LYS A 83146.223 3.638 -7.751 1.00 0.00 C ATOM 1194 CG LYS A 83147.353 3.770 -8.758 1.00 0.00 C ATOM 1195 CD LYS A 83146.881 3.453 -10.168 1.00 0.00 C ATOM 1196 CE LYS A 83147.739 4.151 -11.212 1.00 0.00 C ATOM 1197 NZ LYS A 83148.766 3.239 -11.787 1.00 0.00 N ATOM 1198 H LYS A 83147.796 1.924 -6.735 1.00 0.00 H ATOM 1199 HA LYS A 83147.196 4.615 -6.114 1.00 0.00 H ATOM 1200 1HB LYS A 83145.717 2.701 -7.929 1.00 0.00 H ATOM 1201 2HB LYS A 83145.528 4.449 -7.914 1.00 0.00 H ATOM 1202 1HG LYS A 83147.728 4.782 -8.734 1.00 0.00 H ATOM 1203 2HG LYS A 83148.143 3.085 -8.489 1.00 0.00 H ATOM 1204 1HD LYS A 83146.938 2.386 -10.325 1.00 0.00 H ATOM 1205 2HD LYS A 83145.858 3.782 -10.277 1.00 0.00 H ATOM 1206 1HE LYS A 83147.099 4.504 -12.007 1.00 0.00 H ATOM 1207 2HE LYS A 83148.234 4.991 -10.749 1.00 0.00 H ATOM 1208 1HZ LYS A 83148.971 2.466 -11.121 1.00 0.00 H ATOM 1209 2HZ LYS A 83149.645 3.761 -11.974 1.00 0.00 H ATOM 1210 3HZ LYS A 83148.422 2.831 -12.680 1.00 0.00 H ATOM 1211 N LEUA 84145.250 4.640 -4.605 1.00 0.00 N ATOM 1212 CA LEU A 84144.136 4.675 -3.666 1.00 0.00 C ATOM 1213 C LEU A 84142.808 4.456 -4.384 1.00 0.00 C

ATOM 1214 O LEUA 84141.894 3.832 -3.844 1.00 0.00 O ATOM 1215 CB LEU A 84144.115 6.015 -2.924 1.00 0.00 C ATOM 1216 CG LEU A 84142.921 6.222 -1.990 1.00 0.00 C ATOM 1217 CD1 LEU A 84143.105 5.434 -0.703 1.00 0.00 C ATOM 1218 CD2 LEU A 84142.732 7.702 -1.689 1.00 0.00 C ATOM 1219 H LEU A 84145.833 5.423 -4.683 1.00 0.00 H ATOM 1220 HA LEU A 84144.280 3.880 -2.950 1.00 0.00 H ATOM 1221 1HB LEU A 84145.020 6.091 -2.340 1.00 0.00 H ATOM 1222 2HB LEU A 84144.112 6.807 -3.658 1.00 0.00 H ATOM 1223 HG LEU A 84142.025 5.863 -2.476 1.00 0.00 H ATOM 1224 1HD1 LEU A 84142.152 5.045 -0.380 1.00 0.00 H ATOM 1225 2HD1 LEU A 84143.508 6.082 0.061 1.00 0.00 H ATOM 1226 3HD1 LEU A 84143.789 4.616 -0.878 1.00 0.00 H ATOM 1227 1HD2 LEU A 84142.418 8.215 -2.586 1.00 0.00 H ATOM 1228 2HD2 LEU A 84143.667 8.121 -1.345 1.00 0.00 H ATOM 1229 3HD2 LEU A 84141.981 7.821 -0.924 1.00 0.00 H ATOM 1230 N LYS A 85142.708 4.971 -5.606 1.00 0.00 N ATOM 1231 CA LYS A 85141.491 4.830 -6.398 1.00 0.00 C ATOM 1232 C LYS A 85141.220 3.365 -6.728 1.00 0.00 C ATOM 1233 O LYS A 85140.075 2.975 -6.956 1.00 0.00 O ATOM 1234 CB LYS A 85141.602 5.645 -7.688 1.00 0.00 C ATOM 1235 CG LYS A 85142.793 5.264 -8.549 1.00 0.00 C ATOM 1236 CD LYS A 85143.264 6.434 -9.398 1.00 0.00 C ATOM 1237 CE LYS A 85144.650 6.186 -9.970 1.00 0.00 C ATOM 1238 NZ LYS A 85145.138 7.346 -10.766 1.00 0.00 N ATOM 1239 H LYS A 85143.471 5.458 -5.982 1.00 0.00 H ATOM 1240 HA LYS A 85140.670 5.213 -5.811 1.00 0.00 H ATOM 1241 1HB LYS A 85140.702 5.500 -8.269 1.00 0.00 H ATOM 1242 2HB LYS A 85141.690 6.691 -7.433 1.00 0.00 H ATOM 1243 1HG LYS A 85143.602 4.949 -7.909 1.00 0.00 H ATOM 1244 2HG LYS A 85142.509 4.449 -9.200 1.00 0.00 H

ATOM 1245 1HD LYS A 85142.570 6.576 -10.214 1.00 0.00 H ATOM 1246 2HD LYS A 85143.289 7.323 -8.786 1.00 0.00 H ATOM 1247 1HE LYS A 85145.335 6.008 -9.154 1.00 0.00 H ATOM 1248 2HE LYS A 85144.613 5.314 -10.605 1.00 0.00 H ATOM 1249 1HZ LYS A 85146.175 7.409 -10.708 1.00 0.00 H ATOM 1250 2HZ LYS A 85144.728 8.229 -10.401 1.00 0.00 H ATOM 1251 3HZ LYS A 85144.863 7.236 -11.763 1.00 0.00 H ATOM 1252 N SER A 86142.277 2.559 -6.753 1.00 0.00 N ATOM 1253 CA SER A 86142.146 1.139 -7.057 1.00 0.00 C ATOM 1254 C SER A 86142.102 0.309 -5.777 1.00 0.00 C ATOM 1255 O SER A 86142.605 -0.814 -5.737 1.00 0.00 O ATOM 1256 CB SER A 86143.308 0.676 -7.938 1.00 0.00 C ATOM 1257 OG SER A 86143.567 1.608 -8.973 1.00 0.00 O ATOM 1258 H SER A 86143.165 2.928 -6.563 1.00 0.00 H ATOM 1259 HA SER A 86141.220 0.999 -7.594 1.00 0.00 H ATOM 1260 1HB SER A 86144.197 0.572 -7.334 1.00 0.00 H ATOM 1261 2HB SER A 86143.062 -0.278 -8.382 1.00 0.00 H ATOM 1262 HG SER A 86143.066 1.365 -9.755 1.00 0.00 H ATOM 1263 N CYS A 87141.498 0.868 -4.734 1.00 0.00 N ATOM 1264 CA CYS A 87141.387 0.180 -3.453 1.00 0.00 C ATOM 1265 C CYS A 87139.928 -0.097 -3.109 1.00 0.00 C ATOM 1266 O CYS A 87139.021 0.538 -3.648 1.00 0.00 O ATOM 1267 CB CYS A 87142.036 1.012 -2.345 1.00 0.00 C ATOM 1268 SG CYS A 87143.843 1.034 -2.401 1.00 0.00 S ATOM 1269 H CYS A 87141.116 1.766 -4.828 1.00 0.00 H ATOM 1270 HA CYS A 87141.910 -0.761 -3.537 1.00 0.00 H ATOM 1271 1HB CYS A 87141.693 2.032 -2.424 1.00 0.00 H ATOM 1272 2HB CYS A 87141.740 0.613 -1.386 1.00 0.00 H ATOM 1273 HG CYS A 87144.122 0.522 -3.164 1.00 0.00 H ATOM 1274 N ARG A 88139.706 -1.049 -2.208 1.00 0.00 N ATOM 1275 CA ARG A 88138.356 -1.408 -1.793 1.00 0.00 C

ATOM 1276 C ARG A 88138.267 -1.531 -0.272 1.00 0.00 C ATOM 1277 O ARGA 88139.211 -1.983 0.376 1.00 0.00 O ATOM 1278 CB ARG A 88137.932 -2.723 -2.448 1.00 0.00 C ATOM 1279 CG ARG A 88137.230 -2.538 -3.784 1.00 0.00 C ATOM 1280 CD ARG A 88135.718 -2.566 -3.627 1.00 0.00 C ATOM 1281 NE ARG A 88135.059 -3.157 -4.789 1.00 0.00 N ATOM 1282 CZ ARG A 88135.003 -2.577 -5.985 1.00 0.00 C ATOM 1283 NH1 ARG A 88135.566 -1.391 -6.183 1.00 0.00 N ATOM 1284 NH2 ARG A 88134.382 -3.184 -6.987 1.00 0.00 N ATOM 1285 H ARG A 88140.470 -1.520 -1.812 1.00 0.00 H ATOM 1286 HA ARG A 88137.691 -0.623 -2.119 1.00 0.00 H ATOM 1287 1HB ARG A 88138.810 -3.332 -2.608 1.00 0.00 H ATOM 1288 2HB ARG A 88137.260 -3.244 -1.782 1.00 0.00 H ATOM 1289 1HG ARG A 88137.521 -1.587 -4.204 1.00 0.00 H ATOM 1290 2HG ARG A 88137.529 -3.335 -4.449 1.00 0.00 H ATOM 1291 1HD ARG A 88135.471 -3.146 -2.750 1.00 0.00 H ATOM 1292 2HD ARG A 88135.364 -1.553 -3.501 1.00 0.00 H ATOM 1293 HE ARG A 88134.634 -4.033 -4.672 1.00 0.00 H ATOM 1294 1HH1 ARG A 88136.035 -0.928 -5.431 1.00 0.00 H ATOM 1295 2HH1 ARG A 88135.520 -0.961 -7.084 1.00 0.00 H ATOM 1296 1HH2 ARG A 88133.956 -4.077 -6.844 1.00 0.00 H ATOM 1297 2HH2 ARG A 88134.340 -2.748 -7.887 1.00 0.00 H ATOM 1298 N PRO A 89137.126 -1.131 0.319 1.00 0.00 N ATOM 1299 CA PRO A 89136.924 -1.201 1.769 1.00 0.00 C ATOM 1300 C PRO A 89137.168 -2.603 2.320 1.00 0.00 C ATOM 1301 O PRO A 89136.530 -3.566 1.898 1.00 0.00 O ATOM 1302 CB PRO A 89135.455 -0.807 1.948 1.00 0.00 C ATOM 1303 CG PRO A 89135.126 -0.003 0.740 1.00 0.00 C ATOM 1304 CD PRO A 89135,949 -0.581 -0.377 1.00 0.00 C ATOM 1305 HA PRO A 89137.555 -0.497 2.291 1.00 0.00 H ATOM 1306 1HB PRO A 89134.846 -1.698 2.009 1.00 0.00 H

ATOM 1307 2HB PRO A 89135.343 -0.225 2.851 1.00 0.00 H ATOM 1308 1HG PRO A 89134.074 -0.091 0.515 1.00 0.00 H ATOM 1309 2HG PRO A 89135.390 1.031 0.903 1.00 0.00 H ATOM 1310 1HD PRO A 89135.401 -1.361 -0.886 1.00 0.00 H ATOM 1311 2HD PRO A 89136.239 0.195 -1.072 1.00 0.00 H ATOM 1312 N ASPA 90138.095 -2.707 3.267 1.00 0.00 N ATOM 1313 CA ASPA 90138.422 -3.991 3.877 1.00 0.00 C ATOM 1314 C ASPA 90137.795 -4.110 5.262 1.00 0.00 C ATOM 1315 O ASPA 90138.296 -3.540 6.232 1.00 0.00 O ATOM 1316 CB ASPA 90139.940 -4.160 3.977 1.00 0.00 C ATOM 1317 CG ASPA 90140.365 -5.614 3.896 1.00 0.00 C ATOM 1318 OD1 ASP A 90139.547 -6.492 4.244 1.00 0.00 O ATOM 1319 OD2 ASP A 90141.516 -5.873 3.485 1.00 0.00 O ATOM 1320 H ASPA 90138.570 -1.902 3.563 1.00 0.00 H ATOM 1321 HA ASPA 90138.023 -4.769 3.245 1.00 0.00 H ATOM 1322 1HB ASP A 90140.410 -3.622 3.168 1.00 0.00 H ATOM 1323 2HB ASP A 90140.279 -3.756 4.919 1.00 0.00 H ATOM 1324 N SER A 91136.695 -4.850 5.346 1.00 0.00 N ATOM 1325 CA SER A 91135.997 -5.042 6.613 1.00 0.00 C ATOM 1326 C SER A 91136.378 -6.376 7.247 1.00 0.00 C ATOM 1327 O SER A 91135.575 -6.993 7.947 1.00 0.00 O ATOM 1328 CB SER A 91134.485 -4.978 6.401 1.00 0.00 C ATOM 1329 OG SER A 91133.828 -4.483 7.554 1.00 0.00 O ATOM 1330 H SER A 91136.343 -5.278 4.537 1.00 0.00 H ATOM 1331 HA SER A 91136.293 -4.243 7.277 1.00 0.00 H ATOM 1332 1HB SER A 91134.267 -4.326 5.569 1.00 0.00 H ATOM 1333 2HB SER A 91134.112 -5.970 6.187 1.00 0.00 H ATOM 1334 HG SER A 91133.100 -5.065 7.784 1.00 0.00 H ATOM 1335 N ARG A 92137.608 -6.815 6.999 1.00 0.00 N ATOM 1336 CA ARG A 92138.093 -8.076 7.546 1.00 0.00 C ATOM 1337 C ARG A 92138.164 -8.018 9.069 1.00 0.00 C

ATOM 1338 O ARG A 92137.993 -9.030 9.748 1.00 0.00 O ATOM 1339 CB ARG A 92139.471 -8.409 6.972 1.00 0.00 C ATOM 1340 CG ARG A 92139.416 -9.230 5.695 1.00 0.00 C ATOM 1341 CD ARG A 92139.022 -10.671 5.976 1.00 0.00 C ATOM 1342 NE ARG A 92137.589 -10.891 5.797 1.00 0.00 N ATOM 1343 CZ ARG A 92137.005 -11.048 4.612 1.00 0.00 C ATOM 1344 NH1 ARG A 92137.727 -11.011 3.498 1.00 0.00 N ATOM 1345 NH2 ARG A 92135.696 -11.243 4.538 1.00 0.00 N ATOM 1346 H ARG A 92138.202 -6.278 6.434 1.00 0.00 H ATOM 1347 HA ARG A 92137.398 -8.851 7.260 1.00 0.00 H ATOM 1348 1HB ARG A 92139.992 -7.486 6.760 1.00 0.00 H ATOM 1349 2HB ARG A 92140.030 -8.966 7.709 1.00 0.00 H ATOM 1350 1HG ARG A 92138.688 -8.792 5.028 1.00 0.00 H ATOM 1351 2HG ARG A 92140.390 -9.216 5.227 1.00 0.00 H ATOM 1352 1HD ARG A 92139.562 -11.318 5.300 1.00 0.00 H ATOM 1353 2HD ARG A 92139.290 -10.912 6.994 1.00 0.00 H ATOM 1354 HE ARG A 92137.032 -10.923 6.603 1.00 0.00 H ATOM 1355 1HH1 ARG A 92138.714 -10.864 3.546 1.00 0.00 H ATOM 1356 2HH1 ARG A 92137.282 -11.130 2.611 1.00 0.00 H ATOM 1357 1HH2 ARG A 92135.147 -11.273 5.374 1.00 0.00 H ATOM 1358 2HH2 ARG A 92135.256 -11.362 3.648 1.00 0.00 H ATOM 1359 N PHE A 93138.419 -6.825 9.599 1.00 0.00 N ATOM 1360 CA PHE A 93138.513 -6.636 11.042 1.00 0.00 C ATOM 1361 C PHE A 93137.293 -5.889 11.574 1.00 0.00 C ATOM 1362 O PHE A 93137.385 -5.153 12.557 1.00 0.00 O ATOM 1363 CB PHE A 93139.788 -5.868 11.393 1.00 0.00 C ATOM 1364 CG PHE A 93141.045 -6.662 11.179 1.00 0.00 C ATOM 1365 CD1 PHE A 93141.370 -7.144 9.921 1.00 0.00 C ATOM 1366 CD2 PHE A 93141.902 -6.927 12.236 1.00 0.00 C ATOM 1367 CE1 PHE A 93142.526 -7.875 9.721 1.00 0.00 C ATOM 1368 CE2 PHE A 93143.059 -7.658 12.041 1.00 0.00 C

ATOM 1369 CZ PHE A 93143.371 -8.132 10.782 1.00 0.00 C ATOM 1370 H PHE A 93138.546 -6.056 9.006 1.00 0.00 H ATOM 1371 HA PHE A 93138.552 -7.611 11.502 1.00 0.00 H ATOM 1372 1HB PHE A 93139.848 -4.982 10.780 1.00 0.00 H ATOM 1373 2HB PHE A 93139.751 -5.578 12.433 1.00 0.00 H ATOM 1374 HD1 PHE A 93140.710 -6.943 9.090 1.00 0.00 H ATOM 1375 HD2 PHE A 93141.658 -6.557 13.220 1.00 0.00 H ATOM 1376 HE1 PHE A 93142.768 -8.246 8.735 1.00 0.00 H ATOM 1377 HE2 PHE A 93143.718 -7.857 12.873 1.00 0.00 H ATOM 1378 HZ PHE A 93144.275 -8.704 10.629 1.00 0.00 H ATOM 1379 N ALAA 94136.153 -6.084 10.920 1.00 0.00 N ATOM 1380 CA ALA A 94134.917 -5.429 11.329 1.00 0.00 C ATOM 1381 C ALA A 94134.552 -5.791 12.766 1.00 0.00 C ATOM 1382 O ALAA 94134.390 -6.965 13.099 1.00 0.00 O ATOM 1383 CB ALA A 94133.784 -5.803 10.384 1.00 0.00 C ATOM 1384 H ALA A 94136.142 -6.682 10.143 1.00 0.00 H ATOM 1385 HA ALA A 94135.069 -4.361 11.267 1.00 0.00 H ATOM 1386 1HB ALA A 94134.071 -6.665 9.802 1.00 0.00 H ATOM 1387 2HB ALA A 94133.579 -4.974 9.722 1.00 0.00 H ATOM 1388 3HB ALA A 94132.897 -6.034 10.956 1.00 0.00 H ATOM 1389 N SER A 95134.426 -4.775 13.614 1.00 0.00 N ATOM 1390 CA SER A 95134.082 -4.987 15.014 1.00 0.00 C ATOM 1391 C SER A 95132.642 -4.567 15.290 1.00 0.00 C ATOM 1392 O SER A 95132.089 -3.714 14.596 1.00 0.00 O ATOM 1393 CB SER A 95135.036 -4.205 15.920 1.00 0.00 C ATOM 1394 OG SER A 95136.145 -5.000 16.300 1.00 0.00 O ATOM 1395 H SER A 95134.568 -3.861 13.289 1.00 0.00 H ATOM 1396 HA SER A 95134.184 -6.041 15.225 1.00 0.00 H ATOM 1397 1HB SER A 95135.397 -3.335 15.392 1.00 0.00 H ATOM 1398 2HB SER A 95134.509 -3.893 16.809 1.00 0.00 H ATOM 1399 HG SER A 95136.483 -5.467 15.533 1.00 0.00 H

ATOM 1400 N LEUA 96132.039 -5.172 16.308 1.00 0.00 N ATOM 1401 CA LEU A 96130.663 -4.861 16.676 1.00 0.00 C ATOM 1402 C LEU A 96130.285 -5.533 17.992 1.00 0.00 C ATOM 1403 O LEU A 96129.953 -6.718 18.023 1.00 0.00 O ATOM 1404 CB LEU A 96129.704 -5.307 15.570 1.00 0.00 C ATOM 1405 CG LEU A 96128.495 -4.395 15.355 1.00 0.00 C ATOM 1406 CD1 LEU A 96127.882 -4.636 13.984 1.00 0.00 C ATOM 1407 CD2 LEU A 96127.462 -4.613 16.450 1.00 0.00 C ATOM 1408 H LEUA 96132.531 -5.845 16.825 1.00 0.00 H ATOM 1409 HA LEU A 96130.586 -3.792 16.797 1.00 0.00 H ATOM 1410 1HB LEU A 96130.258 -5.361 14.644 1.00 0.00 H ATOM 1411 2HB LEU A 96129.341 -6.295 15.812 1.00 0.00 H ATOM 1412 HG LEU A 96128.817 -3.364 15.399 1.00 0.00 H ATOM 1413 1HD1 LEU A 96128.625 -5.066 13.328 1.00 0.00 H ATOM 1414 2HD1 LEU A 96127.538 -3.698 13.573 1.00 0.00 H ATOM 1415 3HD1 LEU A 96127.048 -5.315 14.077 1.00 0.00 H ATOM 1416 1HD2 LEU A 96127.130 -5.641 16.431 1.00 0.00 H ATOM 1417 2HD2 LEU A 96126.618 -3.960 16.283 1.00 0.00 H ATOM 1418 3HD2 LEU A 96127.903 -4.395 17.410 1.00 0.00 H ATOM 1419 N GLN A 97130.339 -4.769 19.079 1.00 0.00 N ATOM 1420 CA GLN A 97130.002 -5.290 20.398 1.00 0.00 C ATOM 1421 C GLN A 97130.929 -6.442 20.781 1.00 0.00 C ATOM 1422 O GLN A 97131.595 -7.024 19.925 1.00 0.00 O ATOM 1423 CB GLN A 97128.547 -5.759 20.427 1.00 0.00 C ATOM 1424 CG GLN A 97127.566 -4.676 20.847 1.00 0.00 C ATOM 1425 CD GLN A 97126.204 -4.841 20.203 1.00 0.00 C ATOM 1426 OE1 GLN A 97126.054 -4.681 18.992 1.00 0.00 O ATOM 1427 NE2 GLN A 97125.201 -5.162 21.013 1.00 0.00 N ATOM 1428 H GLN A 97130.611 -3.831 18.990 1.00 0.00 H ATOM 1429 HA GLN A 97130.127 -4.490 21.112 1.00 0.00 H ATOM 1430 1HB GLN A 97128.271 -6.100 19.441 1.00 0.00 H

ATOM 1431 2HB GLN A 97128.459 -6.583 21.121 1.00 0.00 H ATOM 1432 1HG GLN A 97127.447 -4.713 21.920 1.00 0.00 H ATOM 1433 2HG GLN A 97127.970 -3.714 20.564 1.00 0.00 H ATOM 1434 1HE2 GLN A 97125.395 -5.274 21.967 1.00 0.00 H ATOM 1435 2HE2 GLN A 97124.310 -5.275 20.622 1.00 0.00 H ATOM 1436 N PRO A 98130.983 -6.785 22.080 1.00 0.00 N ATOM 1437 CA PRO A 98131.833 -7.874 22.573 1.00 0.00 C ATOM 1438 C PRO A 98131.336 -9.245 22.127 1.00 0.00 C ATOM 1439 O PRO A 98130.179 -9.599 22.350 1.00 0.00 O ATOM 1440 CB PRO A 98131.737 -7.739 24.095 1.00 0.00 C ATOM 1441 CG PRO A 98130.430 -7.067 24.333 1.00 0.00 C ATOM 1442 CD PRO A 98130.221 -6.142 23.166 1.00 0.00 C ATOM 1443 HA PRO A 98132.859 -7.746 22.261 1.00 0.00 H ATOM 1444 1HB PRO A 98131.767 -8.720 24.548 1.00 0.00 H ATOM 1445 2HB PRO A 98132.560 -7.142 24.459 1.00 0.00 H ATOM 1446 1HG PRO A 98129.641 -7.804 24.375 1.00 0.00 H ATOM 1447 2HG PRO A 98130.469 -6.504 25.254 1.00 0.00 H ATOM 1448 1HD PRO A 98129.171 -6.080 22.917 1.00 0.00 H ATOM 1449 2HD PRO A 98130.617 -5.162 23.386 1.00 0.00 H ATOM 1450 N SER A 99132.218 -10.012 21.495 1.00 0.00 N ATOM 1451 CA SER A 99131.868 -11.344 21.017 1.00 0.00 C ATOM 1452 C SER A 99132.957 -12.352 21.371 1.00 0.00 C ATOM 1453 O SER A 99132.687 -13.383 21.987 1.00 0.00 O ATOM 1454 CB SER A 99131.648 -11.324 19.503 1.00 0.00 C ATOM 1455 OG SER A 99132.444 -10.328 18.884 1.00 0.00 O ATOM 1456 H SER A 99133.126 -9.673 21.346 1.00 0.00 H ATOM 1457 HA SER A 99130.950 -11.639 21.502 1.00 0.00 H ATOM 1458 1HB SER A 99131.914 -12.287 19.091 1.00 0.00 H ATOM 1459 2HB SER A 99130.608 -11.119 19.296 1.00 0.00 H ATOM 1460 HG SER A 99131.881 -9.611 18.582 1.00 0.00 H ATOM 1461 N GLY A 100134.190 -12.047 20.978 1.00 0.00 N

ATOM 1462 CA GLY A 100135.300 -12.936 21.263 1.00 0.00 C ATOM 1463 C GLY A 100135.839 -12.759 22.670 1.00 0.00 C ATOM 1464 O GLY A 100135.168 -12.182 23.525 1.00 0.00 O ATOM 1465 H GLY A 100134.346 -11.212 20.491 1.00 0.00 H ATOM 1466 1HA GLY A 100134.970 -13.957 21.141 1.00 0.00 H ATOM 1467 2HA GLY A 100136.095 -12.740 20.557 1.00 0.00 H ATOM 1468 N PRO A 101137.062 -13.248 22.942 1.00 0.00 N ATOM 1469 CA PRO A 101137.680 -13.133 24.267 1.00 0.00 C ATOM 1470 C PRO A 101138.074 -11.697 24.600 1.00 0.00 C ATOM 1471 O PRO A 101137.812 -11.210 25.698 1.00 0.00 O ATOM 1472 CB PRO A 101138.926 -14.015 24.156 1.00 0.00 C ATOM 1473 CG PRO A 101139.252 -14.029 22.703 1.00 0.00 C ATOM 1474 CD PRO A 101137.934 -13.949 21.982 1.00 0.00 C ATOM 1475 HA PRO A 101137.032 -13.516 25.041 1.00 0.00 H ATOM 1476 1HB PRO A 101139.728 -13.586 24.738 1.00 0.00 H ATOM 1477 2HB PRO A 101138.701 -15.007 24.519 1.00 0.00 H ATOM 1478 1HG PRO A 101139.867 -13.176 22.456 1.00 0.00 H ATOM 1479 2HG PRO A 101139.762 -14.947 22.450 1.00 0.00 H ATOM 1480 1HD PRO A 101138.037 -13.382 21.069 1.00 0.00 H ATOM 1481 2HD PRO A 101137.558 -14.940 21.773 1.00 0.00 H ATOM 1482 N SER A 102138.704 -11.024 23.642 1.00 0.00 N ATOM 1483 CA SER A 102139.133 -9.644 23.833 1.00 0.00 C ATOM 1484 C SER A 102139.033 -8.858 22.530 1.00 0.00 C ATOM 1485 O SER A 102140.038 -8.608 21.865 1.00 0.00 O ATOM 1486 CB SER A 102140.569 -9.602 24.359 1.00 0.00 C ATOM 1487 OG SER A 102140.652 -10.160 25.659 1.00 0.00 O ATOM 1488 H SER A 102138.885 -11.467 22.786 1.00 0.00 H ATOM 1489 HA SER A 102138.479 -9.192 24.564 1.00 0.00 H ATOM 1490 1HB SER A 102141.209 -10.168 23.699 1.00 0.00 H ATOM 1491 2HB SER A 102140.907 -8.577 24.398 1.00 0.00 H ATOM 1492 HG SER A 102140.083 -9.667 26.256 1.00 0.00 H

ATOM 1493 N SER A 103137.813 -8.469 22.171 1.00 0.00 N ATOM 1494 CA SER A 103137.575 -7.710 20.947 1.00 0.00 C ATOM 1495 C SER A 103137.853 -8.562 19.712 1.00 0.00 C ATOM 1496 O SER A 103136.932 -8.955 18.997 1.00 0.00 O ATOM 1497 CB SER A 103138.444 -6.450 20.921 1.00 0.00 C ATOM 1498 OG SER A 103137.703 -5.328 20.472 1.00 0.00 O ATOM 1499 H SER A 103137.051 -8.699 22.744 1.00 0.00 H ATOM 1500 HA SER A 103136.535 -7.417 20.938 1.00 0.00 H ATOM 1501 1HB SER A 103138.809 -6.246 21.917 1.00 0.00 H ATOM 1502 2HB SER A 103139.280 -6.603 20.256 1.00 0.00 H ATOM 1503 HG SER A 103137.240 -5.554 19.662 1.00 0.00 H ATOM 1504 N GLY A 104139.130 -8.843 19.468 1.00 0.00 N ATOM 1505 CA GLY A 104139.505 -9.647 18.319 1.00 0.00 C ATOM 1506 C GLY A 104140.109 -8.818 17.205 1.00 0.00 C ATOM 1507 O GLY A 104141.142 -8.158 17.448 1.00 0.00 O ATOM 1508 OXT GLY A 104139.552 -8.828 16.087 1.00 0.00 O ATOM 1509 H GLY A 104139.822 -8.504 20.073 1.00 0.00 H ATOM 1510 1HA GLY A 104140.225 -10.388 18.633 1.00 0.00 H ATOM 1511 2HA GLY A 104138.626 -10.150 17.943 1.00 0.00 H TER 1512 GLY A 104 **ENDMDL**

Three-Dimensional Structure Coordinate Table 3

ATOM 1 N GLY A 1125.212 27.334 -8.433 1.00 0.00 N
ATOM 2 CA GLY A 1126.127 26.226 -8.041 1.00 0.00 C
ATOM 3 C GLY A 1126.734 25.523 -9.238 1.00 0.00 C
ATOM 4 O GLY A 1126.538 24.322 -9.426 1.00 0.00 O
ATOM 5 1H GLY A 1125.466 27.688 -9.377 1.00 0.00 H
ATOM 6 2H GLY A 1125.283 28.114 -7.751 1.00 0.00 H
ATOM 7 3H GLY A 1124.229 26.994 -8.455 1.00 0.00 H
ATOM 8 1HA GLY A 1126.923 26.630 -7.432 1.00 0.00 H

ATOM 9 2HA GLY A 1125.572 25.506 -7.457 1.00 0.00 H ATOM10 N SER A 2127.472 26.272 -10.049 1.00 0.00 N ATOM11 CA SER A 2128.110 25.713 -11.236 1.00 0.00 C ATOM12 C SER A 2129.203 24.723 -10.851 1.00 0.00 C ATOM13 O SER A 2129.120 23.536 -11.169 1.00 0.00 O ATOM14 CB SER A 2128.700 26.831 -12.098 1.00 0.00 C ATOM15 OG SER A 2127.762 27.284 -13.059 1.00 0.00 O ATOM16 H SER A 2127.592 27.223 -9.846 1.00 0.00 H ATOM17 HA SER A 2127.354 25.193 -11.805 1.00 0.00 H ATOM18 1HB SER A 2128.978 27.662 -11.466 1.00 0.00 H ATOM19 2HB SER A 2129.575 26.461 -12.613 1.00 0.00 H ATOM20 HG SER A 2127.770 28.243 -13.087 1.00 0.00 H ATOM21 N SER A 3130.228 25.217 -10.164 1.00 0.00 N ATOM22 CA SER A 3131.338 24.374 -9.734 1.00 0.00 C ATOM23 C SER A 3130.855 23.274 -8.795 1.00 0.00 C ATOM24 O SER A 3130.082 23.528 -7.871 1.00 0.00 O ATOM25 CB SER A 3132.408 25.220 -9.040 1.00 0.00 C ATOM26 OG SER A 3132.727 26.369 -9.806 1.00 0.00 O ATOM27 H SER A 3130.237 26.171 -9.939 1.00 0.00 H ATOM28 HA SER A 3131.767 23.918 -10.613 1.00 0.00 H ATOM29 1HB SER A 3132.043 25.537 -8.075 1.00 0.00 H ATOM30 2HB SER A 3133.302 24.629 -8.910 1.00 0.00 H ATOM31 HG SER A 3132.091 27.063 -9.621 1.00 0.00 H ATOM32 N GLY A 4131.315 22.051 -9.038 1.00 0.00 N ATOM33 CA GLY A 4130.919 20.931 -8.206 1.00 0.00 C ATOM34 C GLY A 4130.532 19.711 -9.020 1.00 0.00 C ATOM35 O GLY A 4129.678 19.791 -9.902 1.00 0.00 O ATOM36 H GLY A 4131.929 21.908 -9.789 1.00 0.00 H ATOM37 1HA GLY A 4131.742 20.670 -7.557 1.00 0.00 H ATOM38 2HA GLY A 4130.076 21.227 -7.599 1.00 0.00 H ATOM39 N SER A 5131.165 18.580 -8.724 1.00 0.00 N

ATOM40 CA SER A 5130.883 17.339 -9.436 1.00 0.00 C ATOM41 C SER A 5129.775 16.553 -8.741 1.00 0.00 C ATOM42 O SER A 5129.529 16.730 -7.548 1.00 0.00 O ATOM43 CB SER A 5132.147 16.483 -9.532 1.00 0.00 C ATOM44 OG SER A 5132.417 15.830 -8.304 1.00 0.00 O ATOM45 H SER A 5131.837 18.580 -8.011 1.00 0.00 H ATOM46 HA SER A 5130.555 17.595 -10.432 1.00 0.00 H ATOM47 1HB SER A 5132.015 15.736 -10.300 1.00 0.00 H ATOM48 2HB SER A 5132.987 17.113 -9.784 1.00 0.00 H ATOM49 HG SER A 5132.762 14.951 -8.477 1.00 0.00 H ATOM50 N SER A 6129.109 15.685 -9.496 1.00 0.00 N ATOM51 CA SER A 6128.028 14.872 -8.952 1.00 0.00 C ATOM52 C SER A 6128.579 13.712 -8.129 1.00 0.00 C ATOM53 O SER A 6129.231 12.814 -8.662 1.00 0.00 O ATOM54 CB SER A 6127.146 14.337 -10.081 1.00 0.00 C ATOM55 OG SER A 6126.755 15.378 -10.960 1.00 0.00 O ATOM56 H SER A 6129.352 15.588 -10.440 1.00 0.00 H ATOM57 HA SER A 6127.431 15.502 -8.309 1.00 0.00 H ATOM58 1HB SER A 6127.695 13.597 -10.644 1.00 0.00 H ATOM59 2HB SER A 6126.260 13.885 -9.661 1.00 0.00 H ATOM60 HG SER A 6127.535 15.778 -11.351 1.00 0.00 H ATOM61 N GLY A 7128.313 13.737 -6.827 1.00 0.00 N ATOM62 CA GLY A 7128.790 12.683 -5.952 1.00 0.00 C ATOM63 C GLY A 7127.664 11.816 -5.421 1.00 0.00 C ATOM64 O GLY A 7127.124 12.079 -4.346 1.00 0.00 O ATOM65 H GLY A 7127.788 14.478 -6.458 1.00 0.00 H ATOM66 1HA GLY A 7129.481 12.060 -6.499 1.00 0.00 H ATOM67 2HA GLY A 7129.308 13.130 -5.116 1.00 0.00 H ATOM68 N LEUA 8127.309 10.783 -6.177 1.00 0.00 N ATOM69 CA LEU A 8126.240 9.875 -5.777 1.00 0.00 C ATOM70 C LEUA 8126.566 9.201 -4.447 1.00 0.00 C

ATOM71 O LEUA 8125.679 8.948 -3.633 1.00 0.00 O ATOM72 CB LEU A 8126.012 8.815 -6.857 1.00 0.00 C ATOM73 CG LEU A 8125.799 9.364 -8.267 1.00 0.00 C ATOM74 CD1 LEU A 8126.357 8.401 -9.305 1.00 0.00 C ATOM75 CD2 LEU A 8124.323 9.626 -8.520 1.00 0.00 C ATOM76 H LEU A 8127.778 10.626 -7.023 1.00 0.00 H ATOM77 HA LEU A 8125.338 10.456 -5.659 1.00 0.00 H ATOM78 1HB LEU A 8126.869 8.158 -6.872 1.00 0.00 H ATOM79 2HB LEU A 8125.141 8.237 -6.585 1.00 0.00 H ATOM80 HG LEU A 8126.328 10.302 -8.366 1.00 0.00 H ATOM81 1HD1 LEU A 8125.688 7.560 -9.412 1.00 0.00 H ATOM82 2HD1 LEU A 8127.328 8.051 -8.985 1.00 0.00 H ATOM83 3HD1 LEU A 8126.453 8.909 -10.253 1.00 0.00 H ATOM84 1HD2 LEU A 8124.119 9.548 -9.578 1.00 0.00 H ATOM85 2HD2 LEU A 8124.069 10.618 -8.177 1.00 0.00 H ATOM86 3HD2 LEU A 8123.731 8.897 -7.986 1.00 0.00 H ATOM87 N ALAA 9127.846 8.913 -4.236 1.00 0.00 N ATOM88 CA ALA A 9128.291 8.269 -3.007 1.00 0.00 C ATOM89 C ALAA 9129.810 8.310 -2.884 1.00 0.00 C ATOM90 O ALAA 9130.425 7.393 -2.339 1.00 0.00 O ATOM91 CB ALA A 9127.794 6.833 -2.955 1.00 0.00 C ATOM92 H ALAA 9128.507 9.141 -4.924 1.00 0.00 H ATOM93 HA ALA A 9127.858 8.805 -2.175 1.00 0.00 H ATOM94 1HB ALA A 9128.506 6.225 -2.415 1.00 0.00 H ATOM95 2HB ALA A 9127.686 6.452 -3.960 1.00 0.00 H ATOM96 3HB ALA A 9126.839 6.800 -2.452 1.00 0.00 H ATOM97 N MET A 10130.412 9.381 -3.394 1.00 0.00 N ATOM98 CA MET A 10131.861 9.542 -3.341 1.00 0.00 C ATOM99 C MET A 10132.281 10.879 -3.949 1.00 0.00 C ATOM 100 O MET A 10132.849 10.924 -5.041 1.00 0.00 O ATOM 101 CB MET A 10132.550 8.392 -4.080 1.00 0.00 C

102 CG META 10131.913 8.058 -5.419 1.00 0.00 C **ATOM** 103 SD META 10132.616 6.579 -6.173 1.00 0.00 S **ATOM** 104 CE MET A 10132.892 7.152 -7.847 1.00 0.00 C **ATOM** 105 H MET A 10129.868 10.079 -3.816 1.00 0.00 H **ATOM** 106 HA MET A 10132.159 9.522 -2.304 1.00 0.00 H **ATOM** 107 1HB MET A 10133.582 8.658 -4.253 1.00 0.00 H **ATOM** 108 2HB MET A 10132.515 7.509 -3.459 1.00 0.00 H ATOM 109 1HG MET A 10130.855 7.900 -5.270 1.00 0.00 H **ATOM** 110 2HG MET A 10132.060 8.892 -6.089 1.00 0.00 H **ATOM** 111 1HE MET A 10133.578 7.985 -7.834 1.00 0.00 H **ATOM** 112 2HE MET A 10131.954 7.464 -8.281 1.00 0.00 H **ATOM** 113 3HE MET A 10133.312 6.350 -8.437 1.00 0.00 H **ATOM** 114 N PRO A 11132.008 11.991 -3.245 1.00 0.00 N **ATOM** 115 CA PRO A 11132.361 13.332 -3.719 1.00 0.00 C ATOM 116 C PRO A 11133.857 13.483 -3.993 1.00 0.00 C **ATOM** 117 O PROA 11134.251 14.000 -5.038 1.00 0.00 O ATOM 118 CB PRO A 11131.929 14.253 -2.573 1.00 0.00 C ATOM 119 CG PRO A 11130.928 13.466 -1.798 1.00 0.00 C ATOM 120 CD PRO A 11131.334 12.027 -1.935 1.00 0.00 C ATOM 121 HA PRO A 11131.811 13.588 -4.613 1.00 0.00 H ATOM 122 1HB PRO A 11132.788 14.507 -1.969 1.00 0.00 H **ATOM** 123 2HB PRO A 11131.492 15.154 -2.979 1.00 0.00 H ATOM 124 1HG PRO A 11130.950 13.764 -0.761 1.00 0.00 H **ATOM** 125 2HG PRO A 11129.942 13.618 -2.212 1.00 0.00 H **ATOM** 126 1HD PRO A 11132.014 11.749 -1.144 1.00 0.00 H ATOM 127 2HD PRO A 11130.465 11.386 -1.931 1.00 0.00 H **ATOM** 128 N PRO A 12134.718 13.035 -3.058 1.00 0.00 N ATOM 129 CA PRO A 12136.168 13.131 -3.217 1.00 0.00 C **ATOM** 130 C PROA 12136.731 12.015 -4.090 1.00 0.00 C **ATOM** 131 O PROA 12137.651 12.234 -4.879 1.00 0.00 O **ATOM** 132 CB PRO A 12136.677 12.999 -1.785 1.00 0.00 C ATOM

133 CG PRO A 12135.676 12.124 -1.112 1.00 0.00 C **ATOM** 134 CD PRO A 12134.349 12.402 -1.774 1.00 0.00 C **ATOM** 135 HA PRO A 12136.461 14.089 -3.621 1.00 0.00 H **ATOM** 136 1HB PRO A 12137.659 12.549 -1.788 1.00 0.00 H **ATOM** 137 2HB PRO A 12136.720 13.974 -1.323 1.00 0.00 H **ATOM** 138 1HG PRO A 12135.949 11.087 -1.246 1.00 0.00 H **ATOM** ATOM 139 2HG PRO A 12135.627 12.365 -0.061 1.00 0.00 H 140 1HD PRO A 12133.815 11.479 -1.940 1.00 0.00 H **ATOM** 141 2HD PRO A 12133.761 13.074 -1.167 1.00 0.00 H **ATOM** 142 N GLY A 13136.173 10.818 -3.944 1.00 0.00 N ATOM 143 CA GLY A 13136.632 9.684 -4.726 1.00 0.00 C - ATOM 144 C GLY A 13136.975 8.487 -3.862 1.00 0.00 C **ATOM** 145 O GLY A 13137.982 7.818 -4.091 1.00 0.00 O **ATOM** 146 H GLY A 13135.443 10.703 -3.300 1.00 0.00 H **ATOM** 147 1HA GLY A 13135.855 9.402 -5.421 1.00 0.00 H **ATOM** 148 2HA GLY A 13137.510 9.976 -5.283 1.00 0.00 H **ATOM** 149 N ASNA 14136.136 8.216 -2.867 1.00 0.00 N **ATOM** 150 CA ASN A 14136.356 7.092 -1.966 1.00 0.00 C **ATOM** 151 C ASN A 14135.123 6.196 -1.901 1.00 0.00 C ATOM 152 O ASN A 14133.991 6.673 -1.989 1.00 0.00 O **ATOM** 153 CB ASN A 14136.708 7.595 -0.565 1.00 0.00 C ATOM 154 CG ASN A 14138.013 8.366 -0.540 1.00 0.00 C **ATOM** 155 OD1 ASN A 14138.027 9.590 -0.676 1.00 0.00 O **ATOM** 156 ND2 ASN A 14139.119 7.653 -0.365 1.00 0.00 N ATOM: 157 H ASN A 14135.350 8.787 -2.737 1.00 0.00 H **ATOM** 158 HA ASN A 14137.185 6.515 -2.350 1.00 0.00 H **ATOM** 159 1HB ASN A 14135.920 8.245 -0.214 1.00 0.00 H ATOM 160 2HB ASN A 14136.797 6.751 0.102 1.00 0.00 H **ATOM** 161 1HD2 ASN A 14139.032 6.682 -0.263 1.00 0.00 H ATOM 162 2HD2 ASN A 14139.977 8.127 -0.344 1.00 0.00 H **ATOM** 163 N SER A 15135.349 4.896 -1.747 1.00 0.00 N **ATOM**

164 CA SER A 15134.257 3.933 -1.670 1.00 0.00 C ATOM 165 C SER A 15133.351 4.234 -0.480 1.00 0.00 C **ATOM** 166 O SER A 15132.125 4.183 -0.592 1.00 0.00 O ATOM 167 CB SER A 15134.808 2.511 -1.559 1.00 0.00 C **ATOM** 168 OG SER A 15133.762 1.569 -1.395 1.00 0.00 O **ATOM** 169 H SER A 15136.274 4.576 -1.683 1.00 0.00 H **ATOM** 170 HA SER A 15133.678 4.015 -2.578 1.00 0.00 H ATOM 171 1HB SER A 15135.357 2.269 -2.456 1.00 0.00 H ATOM 172 2HB SER A 15135.469 2.450 -0.705 1.00 0.00 H **ATOM** 173 HG SER A 15133.843 0.882 -2.061 1.00 0.00 H ATOM 174 N HIS A 16133.961 4.548 0.657 1.00 0.00 N ATOM 175 CA HIS A 16133.209 4.857 1.868 1.00 0.00 C **ATOM** 176 C HIS A 16134.054 5.675 2.839 1.00 0.00 C **ATOM** 177 O HIS A 16133.627 6.726 3.317 1.00 0.00 O ATOM 178 CB HIS A 16132.738 3.568 2.544 1.00 0.00 C **ATOM** 179 CG HIS A 16131.347 3.167 2.163 1.00 0.00 C ATOM 180 ND1 HIS A 16130.235 3.926 2.465 1.00 0.00 N **ATOM** 181 CD2 HIS A 16130.889 2.079 1.500 1.00 0.00 C **ATOM** 182 CE1 HIS A 16129.154 3.321 2.004 1.00 0.00 C ATOM 183 NE2 HIS A 16129.523 2.200 1.414 1.00 0.00 N **ATOM** 184 H HIS A 16134.940 4.572 0.684 1.00 0.00 H ATOM 185 HA HIS A 16132.346 5.439 1.582 1.00 0.00 H **ATOM** 186 1HB HIS A 16133.402 2.762 2.269 1.00 0.00 H ATOM 187 2HB HIS A 16132.765 3.700 3.616 1.00 0.00 H ATOM 188 HD1 HIS A 16130.238 4.780 2.945 1.00 0.00 H **ATOM** 189 HD2 HIS A 16131.487 1.267 1.110 1.00 0.00 H **ATOM** 190 HE1 HIS A 16128.141 3.684 2.094 1.00 0.00 H **ATOM** 191 HE2 HIS A 16128.912 1.519 1.063 1.00 0.00 H **ATOM** 192 N GLYA 17135.256 5.187 3.127 1.00 0.00 N **ATOM** 193 CA GLY A 17136.143 5.884 4.039 1.00 0.00 C **ATOM** ATOM 194 C GLY A 17137.538 5.294 4.059 1.00 0.00 C

195 O GLYA 17138.056 4.942 5.119 1.00 0.00 O ATOM 196 H GLY A 17135.544 4.345 2.716 1.00 0.00 H 197 1HA GLY A 17136.206 6.921 3.740 1.00 0.00 H **ATOM** 198 2HA GLY A 17135.728 5.835 5.036 1.00 0.00 H ATOM ATOM 199 N LEUA 18138.149 5.184 2.883 1.00 0.00 N 200 CA LEU A 18139.492 4.631 2.770 1.00 0.00 C ATOM 201 C LEUA 18140.541 5.657 3.188 1.00 0.00 C ATOM 202 O LEUA 18140.936 6.512 2.396 1.00 0.00 O **ATOM** 203 CB LEU A 18139.758 4.170 1.335 1.00 0.00 C **ATOM** 204 CG LEU A 18138.859 3.033 0.845 1.00 0.00 C **ATOM** 205 CD1 LEU A 18138.767 3.043 -0.673 1.00 0.00 C ATOM 206 CD2 LEU A 18139.378 1.691 1.341 1.00 0.00 C **ATOM** 207 H LEUA 18137.684 5.482 2.074 1.00 0.00 H ATOM 208 HA LEUA 18139.558 3.778 3.429 1.00 0.00 H **ATOM** 209 1HB LEU A 18139.624 5.016 0.677 1.00 0.00 H **ATOM** 210 2HB LEU A 18140.784 3.841 1.268 1.00 0.00 H **ATOM** 211 HG LEU A 18137.863 3.174 1.239 1.00 0.00 H **ATOM** 212 1HD1 LEU A 18139.705 3.382 -1.088 1.00 0.00 H **ATOM** 213 2HD1 LEU A 18137.975 3.707 -0.982 1.00 0.00 H **ATOM** 214 3HD1 LEU A 18138.559 2.043 -1.028 1.00 0.00 H ATOM 215 1HD2 LEU A 18139.928 1.837 2.260 1.00 0.00 H **ATOM** 216 2HD2 LEU A 18140.029 1.260 0.596 1.00 0.00 H ATOM 217 3HD2 LEU A 18138.546 1.028 1.521 1.00 0.00 H **ATOM** 218 N GLUA 19140.986 5.564 4.436 1.00 0.00 N **ATOM** 219 CA GLU A 19141.989 6.485 4.959 1.00 0.00 C ATOM 220 C GLUA 19143.037 5.739 5.779 1.00 0.00 C **ATOM** 221 O GLUA 19142.979 4.517 5.913 1.00 0.00 O ATOM 222 CB GLU A 19141.325 7.562 5.819 1.00 0.00 C ATOM 223 CG GLU A 19140.463 7.001 6.937 1.00 0.00 C ATOM 224 CD GLUA 19139.402 7.979 7.402 1.00 0.00 C ATOM 225 OE1 GLU A 19139.434 8.369 8.589 1.00 0.00 O ATOM

226 OE2 GLU A 19138.541 8.356 6.581 1.00 0.00 O **ATOM** 227 H GLUA 19140.633 4.861 5.019 1.00 0.00 H ATOM 228 HA GLU A 19142.476 6.957 4.119 1.00 0.00 H ATOM 229 1HB GLU A 19142.094 8.179 6.260 1.00 0.00 H **ATOM** 230 2HB GLU A 19140.701 8.176 5.186 1.00 0.00 H ATOM 231 1HG GLU A 19139.974 6.106 6.584 1.00 0.00 H ATOM 232 2HG GLUA 19141.098 6.756 7.776 1.00 0.00 H ATOM ATOM 233 N VALA 20143.994 6.483 6.324 1.00 0.00 N ATOM 234 CA VALA 20145.055 5.891 7.131 1.00 0.00 C 235 C VALA 20144.481 5.136 8.326 1.00 0.00 C ATOM 236 O VALA 20143.631 5.653 9.050 1.00 0.00 O **ATOM** 237 CB VALA 20146.037 6.964 7.639 1.00 0.00 C ATOM 238 CG1 VAL A 20147.209 6.320 8.365 1.00 0.00 C **ATOM** 239 CG2 VAL A 20146.525 7.828 6.485 1.00 0.00 C ATOM 240 H VALA 20143.987 7.452 6.181 1.00 0.00 H ATOM 241 HA VALA 20145.601 5.198 6.508 1.00 0.00 H ATOM 242 HB VALA 20145.515 7.600 8.339 1.00 0.00 H ATOM 243 1HG1 VAL A 20148.077 6.958 8.284 1.00 0.00 H **ATOM** ATOM 244 2HG1 VAL A 20147.425 5.361 7.919 1.00 0.00 H 245 3HG1 VAL A 20146.957 6.185 9.406 1.00 0.00 H ATOM ATOM 246 1HG2 VAL A 20145.737 8.499 6.179 1.00 0.00 H 247 2HG2 VAL A 20146.802 7.196 5.655 1.00 0.00 H ATOM 248 3HG2 VAL A 20147.384 8.402 6.803 1.00 0.00 H **ATOM** 249 N GLY A 21144.950 3.908 8.525 1.00 0.00 N ATOM 250 CA GLY A 21144.472 3.102 9.631 1.00 0.00 C ATOM 251 C GLY A 21143.364 2.152 9.221 1.00 0.00 C ATOM 252 O GLY A 21143.223 1.069 9.789 1.00 0.00 O ATOM ATOM 253 H GLY A 21145.627 3.547 7.913 1.00 0.00 H 254 1HA GLY A 21145.296 2.526 10.025 1.00 0.00 H ATOM 255 2HA GLY A 21144.102 3.757 10.406 1.00 0.00 H ATOM ATOM 256 N SER A 22142.573 2.559 8.232 1.00 0.00 N

257 CA SER A 22141.471 1.736 7.747 1.00 0.00 C **ATOM** 258 C SER A 22141.972 0.673 6.775 1.00 0.00 C **ATOM** 259 O SER A 22142.811 0.948 5.916 1.00 0.00 O **ATOM** 260 CB SER A 22140.417 2.611 7.066 1.00 0.00 C **ATOM** 261 OG SER A 22139.648 3.320 8.022 1.00 0.00 O ATOM 262 H SER A 22142.735 3.432 7.820 1.00 0.00 H ATOM 263 HA SER A 22141.024 1.246 8.598 1.00 0.00 H ATOM 264 1HB SER A 22140.907 3.322 6.417 1.00 0.00 H **ATOM** 265 2HB SER A 22139.756 1.986 6.482 1.00 0.00 H **ATOM** 266 HG SER A 22140.233 3.756 8.644 1.00 0.00 H ATOM 267 N LEUA 23141.454 -0.542 6.915 1.00 0.00 N **ATOM** 268 CA LEUA 23141.848 -1.647 6.049 1.00 0.00 C ATOM 269 C LEUA 23141.271 -1.474 4.649 1.00 0.00 C **ATOM** 270 O LEUA 23140.212 -0.873 4.474 1.00 0.00 O **ATOM** 271 CB LEUA 23141.386 -2.979 6.644 1.00 0.00 C **ATOM** 272 CG LEUA 23142.034 -3.354 7.977 1.00 0.00 C **ATOM** 273 CD1 LEU A 23141.095 -4.216 8.805 1.00 0.00 C ATOM 274 CD2 LEU A 23143.354 -4.074 7.743 1.00 0.00 C ATOM 275 H LEU A 23140.789 -0.700 7.620 1.00 0.00 H **ATOM** 276 HA LEU A 23142.926 -1.648 5.984 1.00 0.00 H ATOM 277 1HB LEU A 23140.316 -2.931 6.788 1.00 0.00 H **ATOM** 278 2HB LEU A 23141.602 -3.761 5.932 1.00 0.00 H **ATOM** 279 HG LEU A 23142.239 -2.452 8.537 1.00 0.00 H ATOM 280 1HD1 LEU A 23140.088 -3.834 8.720 1.00 0.00 H **ATOM** 281 2HD1 LEU A 23141.402 -4.193 9.840 1.00 0.00 H **ATOM** 282 3HD1 LEU A 23141.125 -5.232 8.442 1.00 0.00 H **ATOM** 283 1HD2 LEU A 23143.989 -3.950 8.607 1.00 0.00 H ATOM 284 2HD2 LEU A 23143.843 -3.657 6.874 1.00 0.00 H ATOM 285 3HD2 LEU A 23143.167 -5.125 7.581 1.00 0.00 H ATOM 286 N ALAA 24141.975 -2.007 3.654 1.00 0.00 N ATOM ATOM 287 CA ALAA 24141.532 -1.911 2.269 1.00 0.00 C

- ATOM 288 C ALAA 24142.129 -3.030 1.423 1.00 0.00 C
- ATOM 289 O ALAA 24142.995 -3.774 1.883 1.00 0.00 O
- ATOM 290 CB ALAA 24141.902 -0.554 1.689 1.00 0.00 C
- ATOM 291 H ALA A 24142.811 -2.474 3.858 1.00 0.00 H
- ATOM 292 HA ALA A 24140.455 -1.999 2.256 1.00 0.00 H
- ATOM 293 1HB ALA A 24142.966 -0.395 1.797 1.00 0.00 H
- ATOM 294 2HB ALA A 24141.367 0.221 2.216 1.00 0.00 H
- ATOM 295 3HB ALA A 24141.638 -0.525 0.642 1.00 0.00 H
- ATOM 296 N GLU A 25141.660 -3.144 0.185 1.00 0.00 N
- ATOM 297 CA GLU A 25142.147 -4.174 -0.726 1.00 0.00 C
- ATOM 298 C GLUA 25142.482 -3.580 -2.090 1.00 0.00 C
- ATOM 299 O GLUA 25141.969 -2.524 -2.461 1.00 0.00 O
- ATOM 300 CB GLUA 25141.105 -5.282 -0.880 1.00 0.00 C
- ATOM 301 CG GLU A 25141.622 -6.505 -1.622 1.00 0.00 C
- ATOM 302 CD GLU A 25140.539 -7.537 -1.869 1.00 0.00 C
- ATOM 303 OE1 GLU A 25139.448 -7.152 -2.336 1.00 0.00 O
- ATOM 304 OE2 GLU A 25140.785 -8.732 -1.597 1.00 0.00 O
- ATOM 305 H GLUA 25140.969 -2.522 -0.124 1.00 0.00 H
- ATOM 306 HA GLU A 25143.047 -4.594 -0.299 1.00 0.00 H
- ATOM 307 1HB GLU A 25140.778 -5.594 0.100 1.00 0.00 H
- ATOM 308 2HB GLU A 25140.258 -4.890 -1.424 1.00 0.00 H
- ATOM 309 1HG GLU A 25142.022 -6.190 -2.575 1.00 0.00 H
- ATOM 310 2HG GLU A 25142.407 -6.960 -1.035 1.00 0.00 H
- ATOM 311 N VAL A 26143.346 -4.266 -2.833 1.00 0.00 N
- ATOM 312 CA VAL A 26143.749 -3.806 -4.157 1.00 0.00 C
- ATOM 313 C VALA 26143.397 -4.834 -5.227 1.00 0.00 C
- ATOM 314 O VALA 26143.403 -6.038 -4.971 1.00 0.00 O
- ATOM 315 CB VAL A 26145.261 -3.520 -4.216 1.00 0.00 C
- ATOM 316 CG1 VAL A 26145.630 -2.857 -5.534 1.00 0.00 C
- ATOM 317 CG2 VAL A 26145.688 -2.657 -3.038 1.00 0.00 C
- ATOM 318 H VALA 26143.721 -5.100 -2.482 1.00 0.00 H

319 HA VALA 26143.221 -2.886 -4.366 1.00 0.00 H ATOM 320 HB VALA 26145.788 -4.461 -4.153 1.00 0.00 H ATOM 321 1HG1 VALA 26144.767 -2.343 -5.931 1.00 0.00 H **ATOM** 322 2HG1 VAL A 26145.957 -3.609 -6.236 1.00 0.00 H ATOM **ATOM** 323 3HG1 VAL A 26146.427 -2.146 -5.370 1.00 0.00 H 324 1HG2 VAL A 26145.118 -1.739 -3.039 1.00 0.00 H **ATOM** 325 2HG2 VALA 26146.740 -2.427 -3.122 1.00 0.00 H **ATOM** 326 3HG2 VALA 26145.508 -3.190 -2.117 1.00 0.00 H ATOM 327 N LYS A 27143.090 -4.350 -6.425 1.00 0.00 N **ATOM** 328 CA LYS A 27142.735 -5.226 -7.536 1.00 0.00 C ATOM 329 C LYS A 27143.971 -5.609 -8.343 1.00 0.00 C **ATOM** 330 O LYS A 27144.276 -4.991 -9.362 1.00 0.00 O **ATOM** 331 CB LYS A 27141.708 -4.544 -8.443 1.00 0.00 C **ATOM** 332 CG LYS A 27140.274 -4.963 -8.160 1.00 0.00 C **ATOM** 333 CD LYS A 27139.289 -4.199 -9.032 1.00 0.00 C **ATOM** 334 CE LYS A 27138.175 -5.101 -9.536 1.00 0.00 C ATOM 335 NZ LYS A 27138.653 -6.038 -10.591 1.00 0.00 N ATOM 336 H LYS A 27143.103 -3.380 -6.567 1.00 0.00 H **ATOM** 337 HA LYS A 27142.297 -6.123 -7.123 1.00 0.00 H **ATOM** 338 1HB LYS A 27141.781 -3.475 -8.309 1.00 0.00 H ATOM 339 2HB LYS A 27141.934 -4.786 -9.470 1.00 0.00 H ATOM 340 1HG LYS A 27140.171 -6.019 -8.360 1.00 0.00 H **ATOM** 341 2HG LYS A 27140.050 -4.766 -7.122 1.00 0.00 H **ATOM** 342 1HD LYS A 27138.855 -3.399 -8.451 1.00 0.00 H **ATOM** 343 2HD LYS A 27139.818 -3.785 -9.879 1.00 0.00 H **ATOM** 344 1HE LYS A 27137.790 -5.675 -8.707 1.00 0.00 H **ATOM** 345 2HE LYS A 27137.388 -4.486 -9.945 1.00 0.00 H **ATOM** 346 1HZ LYS A 27139.312 -5.550 -11.231 1.00 0.00 H ATOM 347 2HZ LYS A 27137.849 -6.394 -11.145 1.00 0.00 H **ATOM** 348 3HZ LYS A 27139.145 -6.845 -10.156 1.00 0.00 H ATOM 349 N GLUA 28144.679 -6.635 -7.880 1.00 0.00 N

- ATOM 350 CA GLU A 28145.883 -7.101 -8.559 1.00 0.00 C
- ATOM 351 C GLU A 28145.850 -8.615 -8.743 1.00 0.00 C
- ATOM 352 O GLU A 28144.881 -9.276 -8.371 1.00 0.00 O
- ATOM 353 CB GLU A 28147.129 -6.694 -7.770 1.00 0.00 C
- ATOM 354 CG GLU A 28148.209 -6.054 -8.627 1.00 0.00 C
- ATOM 355 CD GLU A 28147.852 -4.643 -9.054 1.00 0.00 C
- ATOM 356 OE1 GLU A 28147.828 -4.382 -10.276 1.00 0.00 O
- ATOM 357 OE2 GLU A 28147.598 -3.801 -8.168 1.00 0.00 O
- ATOM 358 H GLU A 28144.386 -7.089 -7.063 1.00 0.00 H
- ATOM 359 HA GLU A 28145.915 -6.634 -9.532 1.00 0.00 H
- ATOM 360 1HB GLU A 28146.842 -5.989 -7.005 1.00 0.00 H
- ATOM 361 2HB GLU A 28147.548 -7.573 -7.299 1.00 0.00 H
- ATOM 362 1HG GLU A 28149.127 -6.021 -8.060 1.00 0.00 H
- ATOM 363 2HG GLU A 28148.355 -6.657 -9.511 1.00 0.00 H
- ATOM 364 N ASN A 29146.918 -9.159 -9.319 1.00 0.00 N
- ATOM 365 CA ASN A 29147.013 -10.595 -9.551 1.00 0.00 C
- ATOM 366 C ASN A 29147.022 -11.360 -8.230 1.00 0.00 C
- ATOM 367 O ASN A 29146.158 -12.203 -7.987 1.00 0.00 O
- ATOM 368 CB ASN A 29148.275 -10.920 -10.354 1.00 0.00 C
- ATOM 369 CG ASN A 29147.996 -11.056 -11.838 1.00 0.00 C
- ATOM 370 OD1 ASN A 29147.912 -12.164 -12.367 1.00 0.00 O
- ATOM 371 ND2 ASN A 29147.853 -9.925 -12.519 1.00 0.00 N
- ATOM 372 H ASN A 29147.660 -8.580 -9.594 1.00 0.00 H
- ATOM 373 HA ASN A 29146.146 -10.896 -10.121 1.00 0.00 H
- ATOM 374 1HB ASN A 29148.997 -10.130 -10.214 1.00 0.00 H
- ATOM 375 2HB ASN A 29148.691 -11.852 -9.998 1.00 0.00 H
- ATOM 376 1HD2 ASN A 29147.934 -9.078 -12.031 1.00 0.00 H
- ATOM 377 2HD2 ASN A 29147.672 -9.983 -13.480 1.00 0.00 H
- ATOM 378 N PRO A 30148.002 -11.075 -7.356 1.00 0.00 N
- ATOM 379 CA PRO A 30148.120 -11.741 -6.056 1.00 0.00 C
- ATOM 380 C PRO A 30147.114 -11.205 -5.038 1.00 0.00 C

381 O PRO A 30147.237 -10.072 -4.573 1.00 0.00 O ATOM 382 CB PRO A 30149.546 -11.404 -5.625 1.00 0.00 C **ATOM** 383 CG PRO A 30149.829 -10.088 -6.263 1.00 0.00 C **ATOM** 384 CD PRO A 30149.076 -10.083 -7.567 1.00 0.00 C **ATOM** 385 HA PRO A 30148.011 -12.810 -6.147 1.00 0.00 H **ATOM** 386 1HB PRO A 30149.593 -11.340 -4.546 1.00 0.00 H **ATOM ATOM** 387 2HB PRO A 30150.223 -12.167 -5.977 1.00 0.00 H 388 1HG PRO A 30149.481 -9.289 -5.626 1.00 0.00 H ATOM 389 2HG PRO A 30150.890 -9.989 -6.444 1.00 0.00 H **ATOM** 390 1HD PRO A 30148.662 -9.105 -7.757 1.00 0.00 H ATOM 391 2HD PRO A 30149.722 -10.382 -8.377 1.00 0.00 H **ATOM ATOM** 392 N PRO A 31146.100 -12.014 -4.676 1.00 0.00 N 393 CA PRO A 31145.077 -11.606 -3.707 1.00 0.00 C **ATOM** 394 C PRO A 31145.637 -11.476 -2.293 1.00 0.00 C ATOM 395 O PRO A 31145.647 -12.440 -1.529 1.00 0.00 O **ATOM** 396 CB PRO A 31144.050 -12.738 -3.773 1.00 0.00 C ATOM 397 CG PRO A 31144.818 -13.920 -4.250 1.00 0.00 C **ATOM** 398 CD PRO A 31145.872 -13.382 -5.177 1.00 0.00 C **ATOM** 399 HA PRO A 31144.611 -10.675 -3.994 1.00 0.00 H ATOM **ATOM** 400 1HB PRO A 31143.633 -12.906 -2.791 1.00 0.00 H 401 2HB PRO A 31143.263 -12.474 -4.464 1.00 0.00 H ATOM ATOM 402 1HG PRO A 31145.278 -14.423 -3.411 1.00 0.00 H 403 2HG PRO A 31144.163 -14.596 -4.779 1.00 0.00 H ATOM 404 1HD PRO A 31146.773 -13.973 -5.109 1.00 0.00 H **ATOM** 405 2HD PRO A 31145.507 -13.363 -6.193 1.00 0.00 H ATOM 406 N PHE A 32146.101 -10.278 -1.955 1.00 0.00 N **ATOM** 407 CA PHE A 32146.662 -10.020 -0.634 1.00 0.00 C ATOM **ATOM** 408 C PHE A 32145.773 -9.069 0.160 1.00 0.00 C 409 O PHE A 32144.803 -8.524 -0.368 1.00 0.00 O ATOM 410 CB PHE A 32148.070 -9.434 -0.760 1.00 0.00 C **ATOM** 411 CG PHE A 32148.162 -8.301 -1.742 1.00 0.00 C ATOM

412 CD1 PHE A 32148.899 -8.435 -2.907 1.00 0.00 C ATOM 413 CD2 PHE A 32147.511 -7.102 -1.499 1.00 0.00 C ATOM **ATOM** 414 CE1 PHE A 32148.985 -7.394 -3.813 1.00 0.00 C 415 CE2 PHE A 32147.593 -6.057 -2.400 1.00 0.00 C ATOM ATOM 416 CZ PHE A 32148.331 -6.203 -3.558 1.00 0.00 C 417 H PHE A 32146.065 -9.548 -2.609 1.00 0.00 H ATOM 418 HA PHE A 32146.721 -10.962 -0.109 1.00 0.00 H **ATOM** 419 1HB PHE A 32148.386 -9.064 0.204 1.00 0.00 H **ATOM** 420 2HB PHE A 32148.748 -10.211 -1.083 1.00 0.00 H **ATOM ATOM** 421 HD1 PHE A 32149.409 -9.365 -3.107 1.00 0.00 H 422 HD2 PHE A 32146.933 -6.987 -0.593 1.00 0.00 H **ATOM** 423 HE1 PHE A 32149.563 -7.510 -4.717 1.00 0.00 H **ATOM** 424 HE2 PHE A 32147.082 -5.128 -2.199 1.00 0.00 H **ATOM** 425 HZ PHE A 32148.397 -5.389 -4.264 1.00 0.00 H **ATOM** 426 N TYR A 33146.109 -8.875 1.431 1.00 0.00 N ATOM 427 CA TYR A 33145.340 -7.989 2.298 1.00 0.00 C **ATOM** 428 C TYR A 33146.263 -7.088 3.112 1.00 0.00 C **ATOM** 429 O TYR A 33147.282 -7.538 3.635 1.00 0.00 O **ATOM** 430 CB TYR A 33144.448 -8.807 3.236 1.00 0.00 C ATOM 431 CG TYR A 33143.132 -9.218 2.616 1.00 0.00 C ATOM 432 CD1 TYR A 33142.336 -8.293 1.954 1.00 0.00 C ATOM 433 CD2 TYR A 33142.687 -10.531 2.692 1.00 0.00 C **ATOM** 434 CE1 TYR A 33141.131 -8.664 1.386 1.00 0.00 C **ATOM** 435 CE2 TYR A 33141.485 -10.911 2.126 1.00 0.00 C **ATOM** 436 CZ TYR A 33140.711 -9.974 1.474 1.00 0.00 C **ATOM** 437 OH TYRA 33139.514 -10.348 0.910 1.00 0.00 O ATOM 438 H TYR A 33146.892 -9.337 1.795 1.00 0.00 H ATOM 439 HA TYR A 33144.715 -7.371 1.670 1.00 0.00 H ATOM 440 1HB TYR A 33144.972 -9.705 3.527 1.00 0.00 H **ATOM** 441 2HB TYR A 33144.233 -8.221 4.117 1.00 0.00 H **ATOM** ATOM 442 HD1 TYR A 33142.667 -7.267 1.885 1.00 0.00 H

443 HD2 TYR A 33143.295 -11.264 3.203 1.00 0.00 H ATOM 444 HE1 TYR A 33140.527 -7.930 0.875 1.00 0.00 H ATOM 445 HE2 TYR A 33141.156 -11.937 2.196 1.00 0.00 H ATOM 446 HH TYR A 33139.057 -10.955 1.498 1.00 0.00 H ATOM 447 N GLY A 34145.899 -5.814 3.214 1.00 0.00 N **ATOM** 448 CA GLY A 34146.705 -4.871 3.966 1.00 0.00 C ATOM 449 C GLY A 34145.905 -3.675 4.442 1.00 0.00 C ATOM 450 O GLY A 34144.740 -3.513 4.077 1.00 0.00 O ATOM 451 H GLY A 34145.075 -5.513 2.776 1.00 0.00 H ATOM **ATOM** 452 1HA GLY A 34147.123 -5.375 4.825 1.00 0.00 H 453 2HA GLY A 34147.511 -4.524 3.338 1.00 0.00 H **ATOM** 454 N VALA 35146.531 -2.835 5.261 1.00 0.00 N **ATOM** 455 CA VALA 35145.870 -1.647 5.789 1.00 0.00 C **ATOM** 456 C VALA 35146.552 -0.375 5.292 1.00 0.00 C **ATOM** 457 O VALA 35147.766 -0.345 5.095 1.00 0.00 O **ATOM ATOM** 458 CB VALA 35145.861 -1.649 7.330 1.00 0.00 C 459 CG1 VAL A 35147.281 -1.641 7.878 1.00 0.00 C ATOM 460 CG2 VAL A 35145.069 -0.464 7.864 1.00 0.00 C **ATOM** 461 H VALA 35147.459 -3.018 5.515 1.00 0.00 H ATOM 462 HA VALA 35144.846 -1.653 5.443 1.00 0.00 H ATOM 463 HB VALA 35145.378 -2.556 7.665 1.00 0.00 H ATOM 464 1HG1 VAL A 35147.861 -0.890 7.361 1.00 0.00 H **ATOM** 465 2HG1 VAL A 35147.730 -2.611 7.726 1.00 0.00 H **ATOM** 466 3HG1 VAL A 35147.259 -1.415 8.934 1.00 0.00 H **ATOM** 467 1HG2 VAL A 35144.397 -0.107 7.098 1.00 0.00 H **ATOM** 468 2HG2 VAL A 35145.749 0.326 8.144 1.00 0.00 H **ATOM** 469 3HG2 VAL A 35144.500 -0.772 8.729 1.00 0.00 H ATOM 470 N ILE A 36145.761 0.675 5.093 1.00 0.00 N ATOM 471 CA ILE A 36146.289 1.949 4.620 1.00 0.00 C **ATOM** 472 C ILE A 36147.261 2.548 5.632 1.00 0.00 C ATOM ATOM 473 O ILE A 36147.108 2.361 6.840 1.00 0.00 O

474 CB ILE A 36145.160 2.962 4.345 1.00 0.00 C ATOM 475 CG1 ILE A 36144.100 2.342 3.431 1.00 0.00 C ATOM 476 CG2 ILE A 36145.726 4.232 3.724 1.00 0.00 C **ATOM** 477 CD1 ILE A 36142.962 3.283 3.101 1.00 0.00 C ATOM 478 H ILE A 36144.801 0.591 5.268 1.00 0.00 H **ATOM** 479 HA ILE A 36146.816 1.768 3.695 1.00 0.00 H **ATOM** 480 HB ILE A 36144.704 3.224 5.288 1.00 0.00 H ATOM 481 1HG1 ILE A 36144.564 2.046 2.502 1.00 0.00 H **ATOM ATOM** 482 2HG1 ILE A 36143.683 1.472 3.913 1.00 0.00 H 483 1HG2 ILE A 36146.440 4.677 4.402 1.00 0.00 H **ATOM** 484 2HG2 ILE A 36144.923 4.930 3.538 1.00 0.00 H **ATOM ATOM** 485 3HG2 ILE A 36146.216 3.989 2.794 1.00 0.00 H 486 1HD1 ILE A 36143.360 4.209 2.712 1.00 0.00 H **ATOM** 487 2HD1 ILE A 36142.390 3.485 3.995 1.00 0.00 H ATOM 488 3HD1 ILE A 36142.321 2.827 2.360 1.00 0.00 H **ATOM** 489 N ARG A 37148.260 3.266 5.132 1.00 0.00 N **ATOM** 490 CA ARG A 37149.257 3.890 5.993 1.00 0.00 C **ATOM** ATOM 491 C ARG A 37149.449 5.360 5.629 1.00 0.00 C 492 O ARG A 37149.125 6.251 6.413 1.00 0.00 O **ATOM** 493 CB ARG A 37150.590 3.149 5.885 1.00 0.00 C ATOM 494 CG ARG A 37150.463 1.645 6.063 1.00 0.00 C ATOM 495 CD ARG A 37150.492 1.254 7.532 1.00 0.00 C ATOM 496 NE ARG A 37149.280 1.671 8.234 1.00 0.00 N **ATOM** 497 CZ ARG A 37149.190 1.779 9.558 1.00 0.00 C **ATOM** 498 NH1 ARG A 37150,236 1.502 10.326 1.00 0.00 N **ATOM** 499 NH2 ARG A 37148.049 2.166 10.114 1.00 0.00 N **ATOM** 500 H ARG A 37148.330 3.378 4.161 1.00 0.00 H ATOM 501 HA ARG A 37148.903 3.828 7.011 1.00 0.00 H **ATOM** 502 1HB ARG A 37151.018 3.340 4.912 1.00 0.00 H ATOM 503 2HB ARG A 37151.261 3.524 6.644 1.00 0.00 H **ATOM** 504 1HG ARG A 37149.529 1.318 5.633 1.00 0.00 H **ATOM**

505 2HG ARG A 37151.286 1.161 5.556 1.00 0.00 H ATOM 506 1HD ARG A 37150.587 0.181 7.604 1.00 0.00 H ATOM ATOM 507 2HD ARG A 37151.345 1.722 7.999 1.00 0.00 H 508 HE ARG A 37148.493 1.881 7.691 1.00 0.00 H ATOM 509 1HH1 ARG A 37151.098 1.209 9.913 1.00 0.00 H 510 2HH1 ARG A 37150.161 1.585 11.320 1.00 0.00 H ATOM 511 1HH2 ARG A 37147.259 2.376 9.540 1.00 0.00 H **ATOM** 512 2HH2 ARG A 37147.982 2.247 11.108 1.00 0.00 H ATOM 513 N TRPA 38149.977 5.605 4.434 1.00 0.00 N ATOM 514 CA TRP A 38150.210 6.967 3.968 1.00 0.00 C ATOM 515 C TRPA 38149.461 7.233 2.665 1.00 0.00 C **ATOM** 516 O TRPA 38149.556 6.459 1.712 1.00 0.00 O ATOM 517 CB TRPA 38151.709 7.216 3.772 1.00 0.00 C ATOM 518 CG TRPA 38152.013 8.486 3.032 1.00 0.00 C **ATOM** 519 CD1 TRPA 38152.250 9.716 3.576 1.00 0.00 C ATOM 520 CD2 TRP A 38152.100 8.650 1.612 1.00 0.00 C ATOM 521 NE1 TRP A 38152.480 10.635 2.580 1.00 0.00 N ATOM ATOM 522 CE2 TRP A 38152.395 10.004 1.365 1.00 0.00 C 523 CE3 TRP A 38151.959 7.782 0.525 1.00 0.00 C **ATOM** 524 CZ2 TRP A 38152.550 10.509 0.076 1.00 0.00 C ATOM 525 CZ3 TRP A 38152.114 8.285 -0.753 1.00 0.00 C **ATOM** 526 CH2 TRP A 38152.406 9.637 -0.968 1.00 0.00 C **ATOM** 527 H TRPA 38150.215 4.852 3.852 1.00 0.00 H ATOM 528 HA TRPA 38149.839 7.642 4.724 1.00 0.00 H **ATOM** 529 1HB TRP A 38152.188 7.272 4.739 1.00 0.00 H ATOM 530 2HB TRP A 38152.134 6.395 3.212 1.00 0.00 H ATOM 531 HD1 TRPA 38152.253 9.922 4.636 1.00 0.00 H **ATOM** 532 HE1 TRP A 38152.676 11.585 2.716 1.00 0.00 H ATOM ATOM 533 HE3 TRP A 38151.734 6.737 0.672 1.00 0.00 H 534 HZ2 TRP A 38152.772 11.549 -0.107 1.00 0.00 H ATOM ATOM 535 HZ3 TRP A 38152.009 7.629 -1.604 1.00 0.00 H

536 HH2 TRP A 38152.519 9.986 -1.984 1.00 0.00 H ATOM 537 N ILE A 39148.726 8.338 2.631 1.00 0.00 N ATOM 538 CA ILE A 39147.967 8.719 1.446 1.00 0.00 C ATOM 539 C ILE A 39148.411 10.088 0.940 1.00 0.00 C **ATOM** 540 O ILE A 39148.093 11.113 1.541 1.00 0.00 O ATOM **ATOM** 541 CB ILE A 39146.454 8.753 1.731 1.00 0.00 C 542 CG1 ILE A 39146.012 7.460 2.417 1.00 0.00 C **ATOM** 543 CG2 ILE A 39145.675 8.969 0.442 1.00 0.00 C **ATOM** 544 CD1 ILE A 39144.676 7.574 3.117 1.00 0.00 C **ATOM** 545 H ILEA 39148.697 8.917 3.421 1.00 0.00 H ATOM 546 HA ILE A 39148.154 7.983 0.677 1.00 0.00 H ATOM ATOM 547 HB ILE A 39146.253 9.587 2.386 1.00 0.00 H 548 1HG1 ILE A 39145.933 6.677 1.678 1.00 0.00 H **ATOM** 549 2HG1 ILE A 39146.751 7.181 3.154 1.00 0.00 H **ATOM** 550 1HG2 ILE A 39144.625 8.799 0.623 1.00 0.00 H **ATOM ATOM** 551 2HG2 ILE A 39146.028 8.278 -0.310 1.00 0.00 H 552 3HG2 ILE A 39145.822 9.982 0.098 1.00 0.00 H **ATOM** 553 1HD1 ILE A 39144.179 8.477 2.800 1.00 0.00 H **ATOM** 554 2HD1 ILE A 39144.830 7.604 4.186 1.00 0.00 H **ATOM** 555 3HD1 ILE A 39144.064 6.719 2.866 1.00 0.00 H ATOM 556 N GLY A 40149.152 10.097 -0.164 1.00 0.00 N ATOM 557 CA GLY A 40149.630 11.349 -0.720 1.00 0.00 C **ATOM** 558 C GLYA 40150.140 11.202 -2.140 1.00 0.00 C ATOM 559 O GLY A 40149.996 10.144 -2.755 1.00 0.00 O **ATOM** 560 H GLY A 40149.379 9.250 -0.599 1.00 0.00 H **ATOM** 561 1HA GLY A 40148.823 12.064 -0.713 1.00 0.00 H ATOM 562 2HA GLY A 40150.431 11.721 -0.100 1.00 0.00 H ATOM 563 N GLN A 41150.738 12.268 -2.659 1.00 0.00 N ATOM 564 CA GLN A 41151.275 12.266 -4.014 1.00 0.00 C **ATOM** 565 C GLN A 41152.744 12.682 -4.013 1.00 0.00 C ATOM 566 O GLN A 41153.073 13.816 -3.661 1.00 0.00 O

567 CB GLN A 41150.463 13.213 -4.899 1.00 0.00 C **ATOM** 568 CG GLNA 41148.960 13.014 -4.785 1.00 0.00 C 569 CD GLN A 41148.199 14.324 -4.770 1.00 0.00 C ATOM 570 OE1 GLN A 41148.192 15.042 -3.770 1.00 0.00 O ATOM 571 NE2 GLN A 41147.550 14.643 -5.884 1.00 0.00 N ATOM 572 H GLN A 41150.820 13.080 -2.117 1.00 0.00 H **ATOM** 573 HA GLNA 41151.192 11.264 -4.405 1.00 0.00 H **ATOM** 574 1HB GLN A 41150.692 14.230 -4.618 1.00 0.00 H **ATOM** 575 2HB GLN A 41150.750 13.060 -5.927 1.00 0.00 H **ATOM** 576 1HG GLN A 41148.623 12.428 -5.626 1.00 0.00 H **ATOM** 577 2HG GLN A 41148.750 12.481 -3.869 1.00 0.00 H **ATOM** 578 1HE2 GLN A 41147.599 14.024 -6.642 1.00 0.00 H **ATOM** 579 2HE2 GLN A 41147.049 15.485 -5.903 1.00 0.00 H ATOM 580 N PRO A 42153.655 11.772 -4.405 1.00 0.00 N **ATOM** 581 CA PRO A 42155.092 12.061 -4.440 1.00 0.00 C ATOM 582 C PRO A 42155.420 13.259 -5.326 1.00 0.00 C **ATOM** 583 O PRO A 42154.629 13.637 -6.191 1.00 0.00 O ATOM 584 CB PRO A 42155.706 10.783 -5.022 1.00 0.00 C ATOM 585 CG PRO A 42154.698 9.719 -4.754 1.00 0.00 C **ATOM** 586 CD PRO A 42153.361 10.395 -4.841 1.00 0.00 C ATOM 587 HA PRO A 42155.484 12.233 -3.448 1.00 0.00 H **ATOM** 588 1HB PRO A 42155.874 10.911 -6.081 1.00 0.00 H ATOM 589 2HB PRO A 42156.642 10.573 -4.526 1.00 0.00 H **ATOM** 590 1HG PRO A 42154.776 8.942 -5.499 1.00 0.00 H ATOM 591 2HG PRO A 42154.848 9.311 -3.765 1.00 0.00 H **ATOM** 592 1HD PRO A 42152.996 10.381 -5.857 1.00 0.00 H ATOM 593 2HD PRO A 42152.653 9.922 -4.176 1.00 0.00 H ATOM 594 N PRO A 43156.595 13.876 -5.121 1.00 0.00 N ATOM 595 CA PRO A 43157.024 15.037 -5.905 1.00 0.00 C ATOM 596 C PRO A 43157.402 14.663 -7.333 1.00 0.00 C **ATOM** 597 O PRO A 43158.567 14.392 -7.627 1.00 0.00 O ATOM

598 CB PRO A 43158.249 15.545 -5.146 1.00 0.00 C ATOM 599 CG PRO A 43158.788 14.344 -4.449 1.00 0.00 C ATOM 600 CD PRO A 43157.597 13.489 -4.110 1.00 0.00 C **ATOM ATOM** 601 HA PRO A 43156.264 15.804 -5.924 1.00 0.00 H **ATOM** 602 1HB PRO A 43158.965 15.950 -5.847 1.00 0.00 H 603 2HB PRO A 43157.951 16.307 -4.443 1.00 0.00 H ATOM **ATOM** 604 1HG PRO A 43159.457 13.808 -5.107 1.00 0.00 H 605 2HG PRO A 43159.304 14.642 -3.549 1.00 0.00 H ATOM ATOM 606 1HD PRO A 43157.847 12.442 -4.196 1.00 0.00 H **ATOM** 607 2HD PRO A 43157.244 13.713 -3.114 1.00 0.00 H 608 N GLY A 44156.412 14.650 -8.219 1.00 0.00 N **ATOM** 609 CA GLY A 44156.666 14.309 -9.605 1.00 0.00 C **ATOM** 610 C GLY A 44155.424 13.817 -10.320 1.00 0.00 C ATOM **ATOM** 611 O GLY A 44155.089 14.302 -11.401 1.00 0.00 O 612 H GLY A 44155.503 14.876 -7.929 1.00 0.00 H **ATOM** 613 1HA GLY A 44157.039 15.183 -10.117 1.00 0.00 H ATOM 614 2HA GLY A 44157.418 13.535 -9.641 1.00 0.00 H ATOM 615 N LEUA 45154.738 12.852 -9.716 1.00 0.00 N ATOM 616 CA LEU A 45153.525 12.298 -10.306 1.00 0.00 C ATOM **ATOM** 617 C LEUA 45152.337 12.469 -9.368 1.00 0.00 C 618 O LEUA 45152.290 11.867 -8.297 1.00 0.00 O **ATOM** 619 CB LEU A 45153.722 10.815 -10.630 1.00 0.00 C ATOM **ATOM** 620 CG LEU A 45154.338 9.984 -9.503 1.00 0.00 C 621 CD1 LEU A 45154.029 8.505 -9.697 1.00 0.00 C ATOM **ATOM** 622 CD2 LEU A 45155.842 10.216 -9.432 1.00 0.00 C 623 H LEUA 45155.053 12.507 -8.852 1.00 0.00 H **ATOM** 624 HA LEU A 45153.326 12.833 -11.222 1.00 0.00 H ATOM 625 1HB LEU A 45152.760 10.391 -10.877 1.00 0.00 H ATOM 626 2HB LEU A 45154.364 10.739 -11.495 1.00 0.00 H ATOM 627 HG LEU A 45153.907 10.292 -8.561 1.00 0.00 H ATOM 628 1HD1 LEU A 45153.531 8.361 -10.644 1.00 0.00 H ATOM

- ATOM 629 2HD1 LEU A 45153.386 8.164 -8.898 1.00 0.00 H
- ATOM 630 3HD1 LEU A 45154.949 7.939 -9.684 1.00 0.00 H
- ATOM 631 1HD2 LEU A 45156.072 10.818 -8.566 1.00 0.00 H
- ATOM 632 2HD2 LEU A 45156.170 10.728 -10.324 1.00 0.00 H
- ATOM 633 3HD2 LEU A 45156.351 9.266 -9.355 1.00 0.00 H
- ATOM 634 N ASNA 46151.375 13.292 -9.776 1.00 0.00 N
- ATOM 635 CA ASN A 46150.192 13.528 -8.962 1.00 0.00 C
- ATOM 636 C ASN A 46149.268 12.316 -9.000 1.00 0.00 C
- ATOM 637 O ASN A 46148.624 12.044 -10.013 1.00 0.00 O
- ATOM 638 CB ASN A 46149.446 14.769 -9.454 1.00 0.00 C
- ATOM 639 CG ASN A 46148.709 15.484 -8.339 1.00 0.00 C
- ATOM 640 OD1 ASN A 46147.479 15.539 -8.328 1.00 0.00 O
- ATOM 641 ND2 ASN A 46149.460 16.036 -7.393 1.00 0.00 N
- ATOM 642 H ASN A 46151.462 13.744 -10.641 1.00 0.00 H
- ATOM 643 HA ASN A 46150.513 13.691 -7.944 1.00 0.00 H
- ATOM 644 1HB ASN A 46150.154 15.457 -9.891 1.00 0.00 H
- ATOM 645 2HB ASN A 46148.727 14.474 -10.206 1.00 0.00 H
- ATOM 646 1HD2 ASN A 46150.433 15.953 -7.468 1.00 0.00 H
- ATOM 647 2HD2 ASN A 46149.009 16.505 -6.660 1.00 0.00 H
- ATOM 648 N GLU A 47149.212 11.591 -7.889 1.00 0.00 N
- ATOM 649 CA GLU A 47148.370 10.404 -7.789 1.00 0.00 C
- ATOM 650 C GLU A 47148.235 9.958 -6.339 1.00 0.00 C
- ATOM 651 O GLU A 47149.230 9.655 -5.679 1.00 0.00 O
- ATOM 652 CB GLU A 47148.948 9.266 -8.634 1.00 0.00 C
- ATOM 653 CG GLU A 47150.467 9.182 -8.595 1.00 0.00 C
- ATOM 654 CD GLU A 47151.033 8.332 -9.715 1.00 0.00 C
- ATOM 655 OE1 GLU A 47151.096 8.825 -10.861 1.00 0.00 O
- ATOM 656 OE2 GLU A 47151.415 7.173 -9.446 1.00 0.00 O
- ATOM 657 H GLUA 47149.752 11.859 -7.117 1.00 0.00 H
- ATOM 658 HA GLU A 47147.392 10.660 -8.167 1.00 0.00 H
- ATOM 659 1HB GLU A 47148.550 8.329 -8.275 1.00 0.00 H

- ATOM 660 2HB GLU A 47148.645 9.405 -9.662 1.00 0.00 H
- ATOM 661 1HG GLU A 47150.872 10.179 -8.681 1.00 0.00 H
- ATOM 662 2HG GLU A 47150.768 8.755 -7.650 1.00 0.00 H
- ATOM 663 N VALA 48147.003 9.912 -5.846 1.00 0.00 N
- ATOM 664 CA VALA 48146.751 9.495 -4.473 1.00 0.00 C
- ATOM 665 C VALA 48147.166 8.044 -4.268 1.00 0.00 C
- ATOM 666 O VALA 48146.436 7.121 -4.633 1.00 0.00 O
- ATOM 667 CB VALA 48145.266 9.655 -4.096 1.00 0.00 C
- ATOM 668 CG1 VAL A 48145.057 9.375 -2.61,6 1.00 0.00 C
- ATOM 669 CG2 VAL A 48144.768 11.047 -4.457 1.00 0.00 C
- ATOM 670 H VALA 48146.248 10.161 -6.418 1.00 0.00 H
- ATOM 671 HA VALA 48147.340 10.123 -3.819 1.00 0.00 H
- ATOM 672 HB VALA 48144.693 8.934 -4.661 1.00 0.00 H
- ATOM 673 1HG1 VAL A 48145.200 8.321 -2.425 1.00 0.00 H
- ATOM 674 2HG1 VAL A 48144.055 9.659 -2.334 1.00 0.00 H
- ATOM 675 3HG1 VAL A 48145.769 9.945 -2.037 1.00 0.00 H
- ATOM 676 1HG2 VAL A 48145.443 11.500 -5.168 1.00 0.00 H
- ATOM 677 2HG2 VAL A 48144.724 11.656 -3.566 1.00 0.00 H
- ATOM 678 3HG2 VAL A 48143.783 10.975 -4.893 1.00 0.00 H
- ATOM 679 N LEU A 49148.343 7.846 -3.684 1.00 0.00 N
- ATOM 680 CA LEU A 49148.856 6.506 -3.434 1.00 0.00 C
- ATOM 681 C LEU A 49148.772 6.164 -1.953 1.00 0.00 C
- ATOM 682 O LEU A 49149.439 6.784 -1.124 1.00 0.00 O
- ATOM 683 CB LEU A 49150.304 6.392 -3.915 1.00 0.00 C
- ATOM 684 CG LEUA 49150.503 6.575 -5.421 1.00 0.00 C
- ATOM 685 CD1 LEU A 49151.948 6.937 -5.729 1.00 0.00 C
- ATOM 686 CD2 LEU A 49150.097 5.313 -6.168 1.00 0.00 C
- ATOM 687 H LEUA 49148.880 8.621 -3.416 1.00 0.00 H
- ATOM 688 HA LEUA 49148.246 5.808 -3.988 1.00 0.00 H
- ATOM 689 1HB LEU A 49150.892 7.140 -3.402 1.00 0.00 H
- ATOM 690 2HB LEU A 49150.677 5.416 -3.642 1.00 0.00 H

ATOM 691 HG LEU A 49149.875 7.384 -5.765 1.00 0.00 H ATOM 692 1HD1 LEU A 49151.984 7.547 -6.619 1.00 0.00 H 693 2HD1 LEU A 49152.519 6.035 -5.886 1.00 0.00 H 694 3HD1 LEU A 49152.366 7.487 -4.898 1.00 0.00 H ATOM 695 1HD2 LEU A 49149.362 4.774 -5.589 1.00 0.00 H ATOM 696 2HD2 LEU A 49150.966 4.689 -6.318 1.00 0.00 H **ATOM** 697 3HD2 LEU A 49149.676 5.581 -7.125 1.00 0.00 H ATOM 698 N ALAA 50147.948 5.176 -1.625 1.00 0.00 N **ATOM** 699 CA ALA A 50147.780 4.758 -0.242 1.00 0.00 C ATOM 700 C ALA A 50148.746 3.631 0.112 1.00 0.00 C **ATOM** ATOM 701 O ALAA 50148.657 2.531 -0.433 1.00 0.00 O 702 CB ALAA 50146.342 4.325 0.007 1.00 0.00 C **ATOM** 703 H ALAA 50147.443 4.719 -2.329 1.00 0.00 H ATOM 704 HA ALA A 50147.989 5.610 0.387 1.00 0.00 H **ATOM** ATOM 705 1HB ALAA 50145.712 4.691 -0.789 1.00 0.00 H 706 2HB ALA A 50146.003 4.728 0.949 1.00 0.00 H ATOM **ATOM** 707 3HB ALA A 50146.292 3.246 0.039 1.00 0.00 H 708 N GLYA 51149.668 3.914 1.025 1.00 0.00 N ATOM 709 CA GLY A 51150.637 2.915 1.434 1.00 0.00 C **ATOM** 710 C GLY A 51150.011 1.789 2.232 1.00 0.00 C **ATOM** 711 O GLY A 51149.679 1.961 3.406 1.00 0.00 O **ATOM ATOM** 712 H GLY A 51149.691 4.808 1.425 1.00 0.00 H 713 1HA GLY A 51151.104 2.499 0.553 1.00 0.00 H **ATOM** 714 2HA GLY A 51151.396 3.391 2.039 1.00 0.00 H **ATOM** 715 N LEUA 52149.848 0.634 1.596 1.00 0.00 N **ATOM** 716 CA LEU A 52149.257 -0.524 2.256 1.00 0.00 C **ATOM ATOM** 717 C LEUA 52150.331 -1.381 2.919 1.00 0.00 C 718 O LEUA 52151.450 -1.488 2.418 1.00 0.00 O ATOM 719 CB LEUA 52148.468 -1.365 1.248 1.00 0.00 C ATOM **ATOM** 720 CG LEUA 52147.201 -0.702 0.703 1.00 0.00 C ATOM 721 CD1 LEU A 52146.592 -1.549 -0.403 1.00 0.00 C

722 CD2 LEU A 52146.196 -0.478 1.823 1.00 0.00 C ATOM 723 H LEUA 52150.133 0.558 0.662 1.00 0.00 H ATOM 724 HA LEUA 52148.581 -0.163 3.016 1.00 0.00 H **ATOM** ATOM 725 1HB LEU A 52149.119 -1.592 0.416 1.00 0.00 H 726 2HB LEU A 52148.187 -2.291 1.726 1.00 0.00 H **ATOM** 727 HG LEUA 52147.458 0.260 0.284 1.00 0.00 H ATOM 728 1HD1 LEU A 52146.403 -2.546 -0.032 1.00 0.00 H **ATOM ATOM** 729 2HD1 LEU A 52147.276 -1.599 -1.237 1.00 0.00 H 730 3HD1 LEU A 52145.663 -1.103 -0.726 1.00 0.00 H ATOM 731 1HD2 LEU A 52146.362 -1.202 2.607 1.00 0.00 H ATOM 732 2HD2 LEU A 52145.194 -0.592 1.434 1.00 0.00 H ATOM 733 3HD2 LEU A 52146.316 0.519 2.220 1.00 0.00 H **ATOM** 734 N GLUA 53149.982 -1.988 4.049 1.00 0.00 N **ATOM ATOM** 735 CA GLU A 53150.916 -2.836 4.781 1.00 0.00 C 736 C GLU A 53150.448 -4.287 4.782 1.00 0.00 C **ATOM** 737 O GLUA 53149.515 -4.649 5.499 1.00 0.00 O **ATOM** 738 CB GLUA 53151.069 -2.336 6.219 1.00 0.00 C ATOM 739 CG GLU A 53152.057 -3.146 7.042 1.00 0.00 C **ATOM** ATOM 740 CD GLUA 53151.571 -3.395 8.457 1.00 0.00 C 741 OE1 GLU A 53151.282 -4.563 8.789 1.00 0.00 O **ATOM** 742 OE2 GLU A 53151.482 -2.420 9.234 1.00 0.00 O ATOM 743 H GLUA 53149.075 -1.864 4.398 1.00 0.00 H ATOM ATOM 744 HA GLUA 53151.874 -2.779 4.286 1.00 0.00 H **ATOM** 745 1HB GLU A 53151.407 -1.311 6.198 1.00 0.00 H 746 2HB GLU A 53150.107 -2.379 6.707 1.00 0.00 H **ATOM** 747 1HG GLU A 53152.212 -4.099 6.560 1.00 0.00 H **ATOM** 748 2HG GLU A 53152.994 -2.610 7.088 1.00 0.00 H **ATOM** 749 N LEUA 54151.103 -5.114 3.974 1.00 0.00 N ATOM 750 CA LEUA 54150.754 -6.527 3.881 1.00 0.00 C ATOM 751 C LEUA 54151.046 -7.247 5.194 1.00 0.00 C ATOM 752 O LEUA 54152.057 -6.982 5.846 1.00 0.00 O ATOM

753 CB LEU A 54151.524 -7.191 2.739 1.00 0.00 C **ATOM** 754 CG LEU A 54151.324 -6.552 1.364 1.00 0.00 C **ATOM ATOM** 755 CD1 LEU A 54152.297 -7.140 0.354 1.00 0.00 C 756 CD2 LEU A 54149.889 -6.740 0.895 1.00 0.00 C **ATOM** 757 H LEUA 54151.838 -4.767 3.426 1.00 0.00 H **ATOM** 758 HA LEUA 54149.696 -6.594 3.676 1.00 0.00 H **ATOM ATOM** 759 1HB LEU A 54152.578 -7.160 2.978 1.00 0.00 H 760 2HB LEU A 54151.219 -8.225 2.679 1.00 0.00 H **ATOM** 761 HG LEU A 54151.517 -5.492 1.435 1.00 0.00 H **ATOM** 762 1HD1 LEU A 54152.308 -8.216 0.449 1.00 0.00 H **ATOM** 763 2HD1 LEU A 54153.288 -6.753 0.542 1.00 0.00 H ATOM ATOM 764 3HD1 LEU A 54151.988 -6.870 -0.644 1.00 0.00 H 765 1HD2 LEU A 54149.541 -7.721 1.183 1.00 0.00 H **ATOM** 766 2HD2 LEU A 54149.846 -6.644 -0.180 1.00 0.00 H **ATOM** 767 3HD2 LEU A 54149.260 -5.988 1.349 1.00 0.00 H **ATOM** 768 N GLUA 55150.156 -8.157 5.576 1.00 0.00 N **ATOM** 769 CA GLU A 55150.320 -8.914 6.811 1.00 0.00 C **ATOM ATOM** 770 C GLUA 55151.395 -9.986 6.655 1.00 0.00 C 771 O GLUA 55152.090 -10.325 7.612 1.00 0.00 O **ATOM** 772 CB GLU A 55148.994 -9.562 7.217 1.00 0.00 C **ATOM** 773 CG GLU A 55147.871 -8.562 7.436 1.00 0.00 C **ATOM** 774 CD GLU A 55147.824 -8.042 8.859 1.00 0.00 C **ATOM** 775 OE1 GLU A 55146.921 -8.458 9.615 1.00 0.00 O ATOM 776 OE2 GLU A 55148.691 -7.217 9.219 1.00 0.00 O **ATOM** 777 H GLUA 55149.372 -8.323 5.014 1.00 0.00 H ATOM 778 HA GLU A 55150.625 -8.225 7.584 1.00 0.00 H ATOM 779 1HB GLU A 55148.689 -10.248 6.441 1.00 0.00 H **ATOM** 780 2HB GLU A 55149.142 -10.112 8.134 1.00 0.00 H ATOM 781 1HG GLU A 55148.015 -7.726 6.769 1.00 0.00 H **ATOM** 782 2HG GLU A 55146.930 -9.042 7.213 1.00 0.00 H ATOM ATOM 783 N ASP A 56151.525 -10.513 5.442 1.00 0.00 N

784 CA ASP A 56152.516 -11.547 5.161 1.00 0.00 C **ATOM** ATOM 785 C ASP A 56153.811 -10.931 4.642 1.00 0.00 C **ATOM** 786 O ASPA 56153.807 -10.183 3.665 1.00 0.00 O 787 CB ASP A 56151.967 -12.544 4.140 1.00 0.00 C ATOM 788 CG ASP A 56152.412 -13.965 4.423 1.00 0.00 C ATOM **ATOM** 789 OD1 ASP A 56153.373 -14.428 3.773 1.00 0.00 O ATOM 790 OD2 ASP A 56151.800 -14.618 5.295 1.00 0.00 O 791 H ASPA 56150.941 -10.202 4.719 1.00 0.00 H **ATOM** 792 HA ASP A 56152.723 -12.067 6.085 1.00 0.00 H ATOM 793 1HB ASP A 56150.887 -12.516 4.162 1.00 0.00 H **ATOM** ATOM 794 2HB ASP A 56152.310 -12.268 3.155 1.00 0.00 H 795 N GLUA 57154.919 -11.252 5.303 1.00 0.00 N ATOM 796 CA GLU A 57156.222 -10.731 4.908 1.00 0.00 C ATOM 797 C GLUA 57156.628 -11.260 3.536 1.00 0.00 C **ATOM ATOM** 798 O GLUA 57157.106 -12.388 3.411 1.00 0.00 O 799 CB GLU A 57157.282 -11.108 5.946 1.00 0.00 C ATOM ATOM 800 CG GLU A 57157.377 -10.126 7.102 1.00 0.00 C 801 CD GLU A 57158.593 -10.371 7.975 1.00 0.00 C **ATOM** 802 OE1 GLU A 57158.766 -11.514 8.445 1.00 0.00 O **ATOM** 803 OE2 GLU A 57159.372 -9.418 8.188 1.00 0.00 O **ATOM** 804 H GLUA 57154.858 -11.854 6.074 1.00 0.00 H ATOM ATOM 805 HA GLU A 57156.148 -9.655 4.858 1.00 0.00 H 806 1HB GLU A 57157.044 -12.082 6.347 1.00 0.00 H **ATOM** 807 2HB GLU A 57158.245 -11.154 5.460 1.00 0.00 H **ATOM** ATOM 808 1HG GLU A 57157.436 -9.124 6.703 1.00 0.00 H 809 2HG GLU A 57156.490 -10.219 7.711 1.00 0.00 H ATOM 810 N CYS A 58156.432 -10.439 2.510 1.00 0.00 N **ATOM** 811 CA CYS A 58156.777 -10.825 1.146 1.00 0.00 C ATOM 812 C CYS A 58158.157 -10.301 0.765 1.00 0.00 C ATOM **ATOM** 813 O CYS A 58158.426 -9.103 0.859 1.00 0.00 O 814 CB CYS A 58155.730 -10.297 0.164 1.00 0.00 C

- ATOM 815 SG CYS A 58155.833 -11.026 -1.487 1.00 0.00 S
- ATOM 816 H CYS A 58156.047 -9.553 2.673 1.00 0.00 H
- ATOM 817 HA CYS A 58156.789 -11.903 1.100 1.00 0.00 H
- ATOM 818 1HB CYS A 58154.745 -10.506 0.553 1.00 0.00 H
- ATOM 819 2HB CYS A 58155.851 -9.229 0.060 1.00 0.00 H
- ATOM 820 HG CYS A 58155.366 -10.449 -2.096 1.00 0.00 H
- ATOM 821 N ALA A 59159.031 -11.207 0.335 1.00 0.00 N
- ATOM 822 CA ALA A 59160.383 -10.836 -0.060 1.00 0.00 C
- ATOM 823 C ALA A 59160.374 -10.001 -1.337 1.00 0.00 C
- ATOM 824 O ALAA 59160.036 -10.496 -2.411 1.00 0.00 O
- ATOM 825 CB ALA A 59161.238 -12.081 -0.249 1.00 0.00 C
- ATOM 826 H ALA A 59158.758 -12.146 0.282 1.00 0.00 H
- ATOM 827 HA ALA A 59160.815 -10.250 0.738 1.00 0.00 H
- ATOM 828 1HB ALA A 59161.020 -12.524 -1.210 1.00 0.00 H
- ATOM 829 2HB ALA A 59161.015 -12.792 0.533 1.00 0.00 H
- ATOM 830 3HB ALA A 59162.282 -11.811 -0.205 1.00 0.00 H
- ATOM 831 N GLY A 60160.746 -8.732 -1.209 1.00 0.00 N
- ATOM 832 CA GLY A 60160.773 -7.848 -2.360 1.00 0.00 C
- ATOM 833 C GLY A 60160.174 -6.487 -2.062 1.00 0.00 C
- ATOM 834 O GLY A 60160.550 -5.488 -2.673 1.00 0.00 O
- ATOM 835 H GLY A 60161.005 -8.392 -0.328 1.00 0.00 H
- ATOM 836 1HA GLY A 60161.797 -7.717 -2.677 1.00 0.00 H
- ATOM 837 2HA GLY A 60160.215 -8.306 -3.165 1.00 0.00 H
- ATOM 838 N CYS A 61159.239 -6.449 -1.118 1.00 0.00 N
- ATOM 839 CA CYS A 61158.586 -5.201 -0.739 1.00 0.00 C
- ATOM 840 C CYS A 61159.505 -4.349 0.132 1.00 0.00 C
- ATOM 841 O CYS A 61160.621 -4.755 0.456 1.00 0.00 O
- ATOM 842 CB CYS A 61157.281 -5.490 0.005 1.00 0.00 C
- ATOM 843 SG CYS A 61156.114 -6.515 -0.920 1.00 0.00 S
- ATOM 844 H CYS A 61158.981 -7.280 -0.667 1.00 0.00 H
- ATOM 845 HA CYS A 61158.361 -4.657 -1.644 1.00 0.00 H

- ATOM 846 1HB CYS A 61157.507 -6.002 0.928 1.00 0.00 H
- ATOM 847 2HB CYS A 61156.791 -4.554 0.230 1.00 0.00 H
- ATOM 848 HG CYS A 61155.351 -6.675 -0.360 1.00 0.00 H
- ATOM 849 N THR A 62159.026 -3.168 0.508 1.00 0.00 N
- ATOM 850 CA THR A 62159.805 -2.260 1.342 1.00 0.00 C
- ATOM 851 C THR A 62159.217 -2.171 2.746 1.00 0.00 C
- ATOM 852 O THR A 62158.231 -2.839 3.059 1.00 0.00 O
- ATOM 853 CB THR A 62159.854 -0.868 0.708 1.00 0.00 C
- ATOM 854 OG1 THR A 62158.550 -0.421 0.380 1.00 0.00 O
- ATOM 855 CG2 THR A 62160.689 -0.814 -0.553 1.00 0.00 C
- ATOM 856 H THR A 62158.130 -2.901 0.218 1.00 0.00 H
- ATOM 857 HA THR A 62160.810 -2.650 1.410 1.00 0.00 H
- ATOM 858 HB THR A 62160.282 -0.176 1.418 1.00 0.00 H
- ATOM 859 HG1 THR A 62158.188 -0.974 -0.315 1.00 0.00 H
- ATOM 860 1HG2 THR A 62160.904 -1.819 -0.886 1.00 0.00 H
- ATOM 861 2HG2 THR A 62161.615 -0.296 -0.349 1.00 0.00 H
- ATOM 862 3HG2 THR A 62160.144 -0.288 -1.323 1.00 0.00 H
- ATOM 863 N ASPA 63159.827 -1.342 3.587 1.00 0.00 N
- ATOM 864 CA ASP A 63159.363 -1.166 4.958 1.00 0.00 C
- ATOM 865 C ASP A 63158.671 0.182 5.130 1.00 0.00 C
- ATOM 866 O ASPA 63158.779 0.818 6.178 1.00 0.00 O
- ATOM 867 CB ASP A 63160.536 -1.278 5.934 1.00 0.00 C
- ATOM 868 CG ASPA 63161.601 -0.229 5.680 1.00 0.00 C
- ATOM 869 OD1 ASP A 63162.691 -0.596 5.192 1.00 0.00 O
- ATOM 870 OD2 ASP A 63161.345 0.958 5.968 1.00 0.00 O
- ATOM 871 H ASPA 63160.608 -0.838 3.278 1.00 0.00 H
- ATOM 872 HA ASP A 63158.653 -1.952 5.171 1.00 0.00 H
- ATOM 873 1HB ASP A 63160.170 -1.156 6.942 1.00 0.00 H
- ATOM 874 2HB ASP A 63160.987 -2.255 5.834 1.00 0.00 H
- ATOM 875 N GLY A 64157.960 0.612 4.093 1.00 0.00 N
- ATOM 876 CA GLY A 64157.260 1.882 4.148 1.00 0.00 C

ATOM 877 C GLYA 64158.013 2.990 3.440 1.00 0.00 C 878 O GLYA 64158.125 4.102 3.956 1.00 0.00 O ATOM 879 H GLY A 64157.909 0.062 3.282 1.00 0.00 H ATOM 880 1HA GLY A 64156.291 1.767 3.687 1.00 0.00 H **ATOM** 881 2HA GLY A 64157.123 2.160 5.183 1.00 0.00 H ATOM **ATOM** 882 N THR A 65158.529 2.687 2.253 1.00 0.00 N 883 CA THR A 65159.276 3.667 1.472 1.00 0.00 C **ATOM** 884 C THR A 65158.845 3.638 0.009 1.00 0.00 C **ATOM** 885 O THR A 65158.797 2.578 -0.614 1.00 0.00 O **ATOM** 886 CB THR A 65160.778 3.398 1.578 1.00 0.00 C ATOM **ATOM** 887 OG1 THR A 65161.034 2.006 1.641 1.00 0.00 O 888 CG2 THR A 65161.415 4.039 2.791 1.00 0.00 C ATOM 889 H THR A 65158.406 1.784 1.894 1.00 0.00 H **ATOM** 890 HA THR A 65159.064 4.645 1.877 1.00 0.00 H **ATOM** 891 HB THR A 65161.266 3.793 0.700 1.00 0.00 H ATOM ATOM 892 HG1 THR A 65160.910 1.618 0.773 1.00 0.00 H 893 1HG2 THR A 65162.234 3.423 3.135 1.00 0.00 H **ATOM** 894 2HG2 THR A 65160.681 4.133 3.577 1.00 0.00 H **ATOM** 895 3HG2 THR A 65161.788 5.018 2.527 1.00 0.00 H ATOM 896 N PHE A 66158.530 4.811 -0.533 1.00 0.00 N **ATOM** ATOM 897 CA PHE A 66158.103 4.921 -1.923 1.00 0.00 C **ATOM** 898 C PHE A 66159.010 5.872 -2.697 1.00 0.00 C 899 O PHE A 66159.157 7.039 -2.334 1.00 0.00 O **ATOM** 900 CB PHE A 66156.655 5.406 -1.996 1.00 0.00 C **ATOM ATOM** 901 CG PHE A 66155.978 5.083 -3.298 1.00 0.00 C 902 CD1 PHE A 66155.722 3.769 -3.654 1.00 0.00 C **ATOM** 903 CD2 PHE A 66155.598 6.094 -4.166 1.00 0.00 C ATOM 904 CE1 PHE A 66155.100 3.468 -4.851 1.00 0.00 C ATOM 905 CE2 PHE A 66154.976 5.801 -5.364 1.00 0.00 C **ATOM** 906 CZ PHE A 66154.726 4.486 -5.707 1.00 0.00 C ATOM 907 H PHE A 66158.588 5.621 0.015 1.00 0.00 H ATOM

908 HA PHE A 66158.168 3.939 -2.369 1.00 0.00 H **ATOM ATOM** 909 1HB PHE A 66156.086 4.943 -1.204 1.00 0.00 H 910 2HB PHE A 66156.635 6.478 -1.867 1.00 0.00 H **ATOM** 911 HD1 PHE A 66156.014 2.973 -2.985 1.00 0.00 H **ATOM** 912 HD2 PHE A 66155.792 7.123 -3.898 1.00 0.00 H **ATOM** ATOM 913 HE1 PHE A 66154.907 2.440 -5.117 1.00 0.00 H 914 HE2 PHE A 66154.684 6.598 -6.032 1.00 0.00 H ATOM ATOM 915 HZ PHE A 66154.240 4.254 -6.643 1.00 0.00 H 916 N ARG A 67159.615 5.366 -3.767 1.00 0.00 N ATOM **ATOM** 917 CA ARG A 67160.508 6.172 -4.592 1.00 0.00 C **ATOM** 918 C ARG A 67161.689 6.684 -3.776 1.00 0.00 C 919 O ARG A 67162.217 7.765 -4.039 1.00 0.00 O ATOM 920 CB ARG A 67159.746 7.348 -5.204 1.00 0.00 C ATOM ATOM 921 CG ARG A 67158.677 6.930 -6.200 1.00 0.00 C 922 CD ARG A 67158.317 8.067 -7.143 1.00 0.00 C ATOM ATOM 923 NE ARG A 67159.015 7.958 -8.422 1.00 0.00 N 924 CZ ARG A 67159.160 8.970 -9.274 1.00 0.00 C ATOM 925 NH1 ARG A 67158.658 10.165 -8.989 1.00 0.00 N **ATOM** 926 NH2 ARG A 67159.808 8.786 -10.417 1.00 0.00 N ATOM 927 H ARG A 67159.458 4.429 -4.006 1.00 0.00 H ATOM ATOM 928 HA ARG A 67160.881 5.543 -5.387 1.00 0.00 H ATOM 929 1HB ARG A 67159.271 7.906 -4.411 1.00 0.00 H 930 2HB ARG A 67160.449 7.991 -5.714 1.00 0.00 H ATOM 931 1HG ARG A 67159.045 6.097 -6.780 1.00 0.00 H **ATOM** 932 2HG ARG A 67157.792 6.629 -5.657 1.00 0.00 H ATOM 933 1HD ARG A 67157.253 8.045 -7.322 1.00 0.00 H ATOM 934 2HD ARG A 67158.585 9.003 -6.675 1.00 0.00 H ATOM 935 HE ARG A 67159.396 7.087 -8.657 1.00 0.00 H ATOM **ATOM** 936 1HH1 ARG A 67158.168 10.311 -8.129 1.00 0.00 H 937 2HH1 ARG A 67158.771 10.921 -9.634 1.00 0.00 H ATOM ATOM 938 1HH2 ARG A 67160.188 7.888 -10.637 1.00 0.00 H

- ATOM 939 2HH2 ARG A 67159.917 9.546 -11.058 1.00 0.00 H
- ATOM 940 N GLY A 68162.100 5.902 -2.783 1.00 0.00 N
- ATOM 941 CA GLY A 68163.216 6.295 -1.942 1.00 0.00 C
- ATOM 942 C GLY A 68162.847 7.392 -0.963 1.00 0.00 C
- ATOM 943 O GLY A 68163.696 8.189 -0.564 1.00 0.00 O
- ATOM 944 H GLY A 68161.641 5.052 -2.619 1.00 0.00 H
- ATOM 945 1HA GLY A 68163.556 5.433 -1.389 1.00 0.00 H
- ATOM 946 2HA GLY A 68164.020 6.645 -2.572 1.00 0.00 H
- ATOM 947 N THR A 69161.577 7.433 -0.576 1.00 0.00 N
- ATOM 948 CA THR A 69161.096 8.441 0.363 1.00 0.00 C
- ATOM 949 C THR A 69160.235 7.806 1.449 1.00 0.00 C
- ATOM 950 O THR A 69159.141 7.310 1.178 1.00 0.00 O
- ATOM 951 CB THR A 69160.297 9.515 -0.375 1.00 0.00 C
- ATOM 952 OG1 THR A 69160.987 9.948 -1.533 1.00 0.00 O
- ATOM 953 CG2 THR A 69160.010 10.737 0.472 1.00 0.00 C
- ATOM 954 H THR A 69160.947 6.771 -0.928 1.00 0.00 H
- ATOM 955 HA THR A 69161.957 8.900 0.825 1.00 0.00 H
- ATOM 956 HB THR A 69159.349 9.096 -0.682 1.00 0.00 H
- ATOM 957 HG1 THR A 69161.176 9.193 -2.095 1.00 0.00 H
- ATOM 958 1HG2 THR A 69159.249 11.336 -0.006 1.00 0.00 H
- ATOM 959 2HG2 THR A 69160.913 11.319 0.579 1.00 0.00 H
- ATOM 960 3HG2 THR A 69159.665 10.425 1.447 1.00 0.00 H
- ATOM 961 N ARG A 70160.735 7.825 2.680 1.00 0.00 N
- ATOM 962 CA ARG A 70160.011 7.251 3.809 1.00 0.00 C
- ATOM 963 C ARG A 70158.731 8.032 4.087 1.00 0.00 C
- ATOM 964 O ARG A 70158.765 9.242 4.308 1.00 0.00 O
- ATOM 965 CB ARG A 70160.897 7.239 5.057 1.00 0.00 C
- ATOM 966 CG ARG A 70160.228 6.616 6.272 1.00 0.00 C
- ATOM 967 CD ARG A 70160.684 7.279 7.561 1.00 0.00 C
- ATOM 968 NE ARG A 70162.045 6.890 7.924 1.00 0.00 N
- ATOM 969 CZ ARG A 70162.802 7.562 8.789 1.00 0.00 C

ATOM 970 NH1 ARG A 70162.336 8.654 9.381 1.00 0.00 N 971 NH2 ARG A 70164.028 7.139 9.064 1.00 0.00 N ATOM **ATOM** 972 H ARG A 70161.612 8.235 2.834 1.00 0.00 H 973 HA ARG A 70159.751 6.235 3.553 1.00 0.00 H **ATOM ATOM** 974 1HB ARG A 70161.795 6.681 4.842 1.00 0.00 H **ATOM** 975 2HB ARG A 70161.166 8.256 5.303 1.00 0.00 H 976 1HG ARG A 70159.158 6.731 6.180 1.00 0.00 H **ATOM** 977 2HG ARG A 70160.477 5.566 6.309 1.00 0.00 H ATOM 978 1HD ARG A 70160.650 8.351 7.431 1.00 0.00 H **ATOM ATOM** 979 2HD ARG A 70160.013 6.992 8.356 1.00 0.00 H 980 HE ARG A 70162.414 6.086 7.502 1.00 0.00 H **ATOM** 981 1HH1 ARG A 70161.412 8.979 9.178 1.00 0.00 H **ATOM** 982 2HH1 ARG A 70162.909 9.154 10.030 1.00 0.00 H **ATOM** 983 1HH2 ARG A 70164.384 6.316 8.621 1.00 0.00 H **ATOM** ATOM 984 2HH2 ARG A 70164.597 7.643 9.714 1.00 0.00 H **ATOM** 985 N TYR A 71157.602 7.330 4.076 1.00 0.00 N 986 CA TYR A 71156.310 7.957 4.327 1.00 0.00 C ATOM 987 C TYR A 71155.770 7.560 5.696 1.00 0.00 C **ATOM** 988 O TYR A 71155.270 8.400 6.446 1.00 0.00 O ATOM 989 CB TYR A 71155.309 7.566 3.238 1.00 0.00 C **ATOM** 990 CG TYR A 71155.424 8.400 1.981 1.00 0.00 C ATOM 991 CD1 TYR A 71155.529 9.784 2.050 1.00 0.00 C **ATOM** 992 CD2 TYR A 71155.426 7.802 0.727 1.00 0.00 C ATOM 993 CE1 TYR A 71155.635 10.548 0.905 1.00 0.00 C **ATOM** 994 CE2 TYR A 71155.532 8.561 -0.424 1.00 0.00 C **ATOM ATOM** 995 CZ TYR A 71155.635 9.933 -0.330 1.00 0.00 C 996 OH TYR A 71155.740 10.691 -1.473 1.00 0.00 O **ATOM** 997 H TYR A 71157.639 6.368 3.893 1.00 0.00 H ATOM 998 HA TYR A 71156.451 9.028 4.306 1.00 0.00 H ATOM 999 1HB TYR A 71155.468 6.533 2.966 1.00 0.00 H ATOM ATOM 1000 2HB TYR A 71154.306 7.681 3.623 1.00 0.00 H

ATOM 1001 HD1 TYR A 71155.529 10.262 3.018 1.00 0.00 H ATOM 1002 HD2 TYR A 71155.344 6.728 0.657 1.00 0.00 H ATOM 1003 HE1 TYR A 71155.716 11.623 0.978 1.00 0.00 H ATOM 1004 HE2 TYR A 71155.531 8.078 -1.390 1.00 0.00 H ATOM 1005 HH TYR A 71156.629 10.616 -1.827 1.00 0.00 H ATOM 1006 N PHE A 72155.873 6.274 6.017 1.00 0.00 N ATOM 1007 CA PHE A 72155.395 5.765 7.298 1.00 0.00 C ATOM 1008 C PHE A 72156.315 4.669 7.825 1.00 0.00 C ATOM 1009 O PHE A 72157.106 4.095 7.077 1.00 0.00 O ATOM 1010 CB PHE A 72153,969 5,226 7,156 1,00 0,00 C ATOM 1011 CG PHE A 72153.833 4.157 6.110 1.00 0.00 C ATOM 1012 CD1 PHE A 72153.929 2.818 6.453 1.00 0.00 C ATOM 1013 CD2 PHE A 72153.609 4.491 4.785 1.00 0.00 C ATOM 1014 CE1 PHE A 72153.804 1.832 5.493 1.00 0.00 C ATOM 1015 CE2 PHE A 72153.483 3.510 3.820 1.00 0.00 C ATOM 1016 CZ PHE A 72153.581 2.178 4.174 1.00 0.00 C ATOM 1017 H PHE A 72156.281 5.653 5.379 1.00 0.00 H ATOM 1018 HA PHE A 72155.392 6.585 8.001 1.00 0.00 H ATOM 1019 1HB PHE A 72153.655 4.809 8.101 1.00 0.00 H ATOM 1020 2HB PHE A 72153.311 6.039 6.890 1.00 0.00 H ATOM 1021 HD1 PHE A 72154.104 2.546 7.484 1.00 0.00 H ATOM 1022 HD2 PHE A 72153.533 5.532 4.507 1.00 0.00 H ATOM 1023 HE1 PHE A 72153.881 0.792 5.773 1.00 0.00 H ATOM 1024 HE2 PHE A 72153.309 3.784 2.789 1.00 0.00 H ATOM 1025 HZ PHE A 72153.483 1.410 3.423 1.00 0.00 H ATOM 1026 N THR A 73156.207 4.384 9.119 1.00 0.00 N ATOM 1027 CA THR A 73157.029 3.357 9.747 1.00 0.00 C ATOM 1028 C THR A 73156.250 2.054 9.899 1.00 0.00 C ATOM 1029 O THR A 73155.248 1.997 10.611 1.00 0.00 O ATOM 1030 CB THR A 73157.520 3.832 11.114 1.00 0.00 C ATOM 1031 OG1 THR A 73156.507 4.562 11.785 1.00 0.00 O

ATOM 1032 CG2 THR A 73158.746 4.716 11.036 1.00 0.00 C ATOM 1033 H THR A 73155.558 4.877 9.665 1.00 0.00 H ATOM 1034 HA THR A 73157.882 3.180 9.110 1.00 0.00 H ATOM 1035 HB THR A 73157.771 2.969 11.716 1.00 0.00 H ATOM 1036 HG1 THR A 73156.474 4.291 12.706 1.00 0.00 H ATOM 1037 1HG2 THR A 73159.529 4.199 10.501 1.00 0.00 H ATOM 1038 2HG2 THR A 73159.086 4.949 12.034 1.00 0.00 H ATOM 1039 3HG2 THR A 73158.498 5.630 10.517 1.00 0.00 H ATOM 1040 N CYS A 74156.717 1.009 9.222 1.00 0.00 N ATOM 1041 CA CYS A 74156.065 -0.294 9.281 1.00 0.00 C ATOM 1042 C CYS A 74157.095 -1.417 9.320 1.00 0.00 C ATOM 1043 O CYS A 74158.301 -1.169 9.289 1.00 0.00 O ATOM 1044 CB CYS A 74155.136 -0.478 8.080 1.00 0.00 C ATOM 1045 SG CYS A 74153.445 0.096 8.360 1.00 0.00 S ATOM 1046 H CYS A 74157.521 1.117 8.670 1.00 0.00 H ATOM 1047 HA CYS A 74155.478 -0.329 10.188 1.00 0.00 H ATOM 1048 1HB CYS A 74155.534 0.072 7.241 1.00 0.00 H ATOM 1049 2HB CYS A 74155.091 -1.527 7.828 1.00 0.00 H ATOM 1050 HG CYS A 74153.194 -0.147 9.254 1.00 0.00 H ATOM 1051 N ALA A 75156.613 -2.654 9.386 1.00 0.00 N ATOM 1052 CA ALA A 75157.492 -3.816 9.428 1.00 0.00 C ATOM 1053 C ALAA 75158.208 -4.011 8.096 1.00 0.00 C ATOM 1054 O ALAA 75157.739 -3.552 7.055 1.00 0.00 O ATOM 1055 CB ALA A 75156.700 -5.062 9.791 1.00 0.00 C ATOM 1056 H ALAA 75155.642 -2.787 9.407 1.00 0.00 H ATOM 1057 HA ALA A 75158.229 -3.648 10.200 1.00 0.00 H ATOM 1058 1HB ALA A 75157.137 -5.921 9.302 1.00 0.00 H ATOM 1059 2HB ALA A 75155.676 -4.945 9.467 1.00 0.00 H ATOM 1060 3HB ALA A 75156.725 -5.206 10.861 1.00 0.00 H ATOM 1061 N LEUA 76159.347 -4.695 8.137 1.00 0.00 N ATOM 1062 CA LEU A 76160.129 -4.952 6.933 1.00 0.00 C

ATOM 1063 C LEU A 76159.419 -5.953 6.027 1.00 0.00 C ATOM 1064 O LEUA 76158.846 -6.934 6.499 1.00 0.00 O ATOM 1065 CB LEU A 76161.518 -5.476 7.303 1.00 0.00 C ATOM 1066 CG LEUA 76162.487 -4.420 7.837 1.00 0.00 C ATOM 1067 CD1 LEU A 76163.413 -5.024 8.882 1.00 0.00 C ATOM 1068 CD2 LEU A 76163.291 -3.812 6.698 1.00 0.00 C ATOM 1069 H LEU A 76159.669 -5.036 8.997 1.00 0.00 H ATOM 1070 HA LEU A 76160.236 -4.017 6.402 1.00 0.00 H ATOM 1071 1HB LEU A 76161.401 -6.242 8.056 1.00 0.00 H ATOM 1072 2HB LEU A 76161.956 -5.923 6.425 1.00 0.00 H ATOM 1073 HG LEUA 76161.923 -3.629 8.309 1.00 0.00 H ATOM 1074 1HD1 LEU A 76163.579 -6.067 8.655 1.00 0.00 H ATOM 1075 2HD1 LEU A 76162.961 -4.934 9.858 1.00 0.00 H ATOM 1076 3HD1 LEU A 76164.357 -4.499 8.873 1.00 0.00 H ATOM 1077 1HD2 LEU A 76162.802 -2.913 6.350 1.00 0.00 H ATOM 1078 2HD2 LEU A 76163.359 -4.522 5.886 1.00 0.00 H ATOM 1079 3HD2 LEU A 76164.284 -3.568 7.046 1.00 0.00 H ATOM 1080 N LYS A 77159.463 -5.699 4.723 1.00 0.00 N ATOM 1081 CA LYS A 77158.826 -6.579 3.751 1.00 0.00 C ATOM 1082 C LYS A 77157.321 -6.654 3.991 1.00 0.00 C ATOM 1083 O LYS A 77156.714 -7.719 3.867 1.00 0.00 O ATOM 1084 CB LYS A 77159.436 -7.980 3.821 1.00 0.00 C ATOM 1085 CG LYS A 77160.953 -7.988 3.712 1.00 0.00 C ATOM 1086 CD LYS A 77161.411 -7.675 2.296 1.00 0.00 C ATOM 1087 CE LYS A 77162.908 -7.415 2.240 1.00 0.00 C ATOM 1088 NZ LYS A 77163.667 -8.625 1.820 1.00 0.00 N ATOM 1089 H LYS A 77159.937 -4.902 4.408 1.00 0.00 H ATOM 1090 HA LYS A 77159.002 -6.168 2.768 1.00 0.00 H ATOM 1091 1HB LYS A 77159.163 -8.433 4.762 1.00 0.00 H ATOM 1092 2HB LYS A 77159.036 -8.576 3.014 1.00 0.00 H ATOM 1093 1HG LYS A 77161.357 -7.245 4.383 1.00 0.00 H

ATOM 1094 2HG LYS A 77161.319 -8.966 3.991 1.00 0.00 H ATOM 1095 1HD LYS A 77161.177 -8.513 1.658 1.00 0.00 H ATOM 1096 2HD LYS A 77160.888 -6.797 1.945 1.00 0.00 H ATOM 1097 1HE LYS A 77163.096 -6.620 1.534 1.00 0.00 H ATOM 1098 2HE LYS A 77163.244 -7.112 3.221 1.00 0.00 H ATOM 1099 1HZ LYS A 77163.116 -9.483 2.031 1.00 0.00 H ATOM 1100 2HZ LYS A 77164.572 -8.674 2.329 1.00 0.00 H ATOM 1101 3HZ LYS A 77163.857 -8.590 0.798 1.00 0.00 H ATOM 1102 N LYS A 78156.724 -5.518 4.334 1.00 0.00 N ATOM 1103 CA LYS A 78155.290 -5.455 4.591 1.00 0.00 C ATOM 1104 C LYS A 78154.730 -4.086 4.219 1.00 0.00 C ATOM 1105 O LYS A 78153.888 -3.534 4.928 1.00 0.00 O ATOM 1106 CB LYS A 78155.001 -5.755 6.063 1.00 0.00 C ATOM 1107 CG LYS A 78155.529 -7.104 6.524 1.00 0.00 C ATOM 1108 CD LYS A 78155.130 -7.398 7.961 1.00 0.00 C ATOM 1109 CE LYS A 78153.930 -8.331 8.026 1.00 0.00 C ATOM 1110 NZ LYS A 78152.998 -7.961 9.126 1.00 0.00 N ATOM 1111 H LYS A 78157.261 -4.702 4.417 1.00 0.00 H ATOM 1112 HA LYS A 78154.811 -6.205 3.980 1.00 0.00 H ATOM 1113 1HB LYS A 78155.457 -4.988 6.671 1.00 0.00 H ATOM 1114 2HB LYS A 78153,932 -5.739 6.219 1.00 0.00 H ATOM 1115 1HG LYS A 78155.126 -7.875 5.884 1.00 0.00 H ATOM 1116 2HG LYS A 78156.607 -7.101 6.452 1.00 0.00 H ATOM 1117 1HD LYS A 78155.962 -7.864 8.468 1.00 0.00 H ATOM 1118 2HD LYS A 78154.879 -6.470 8.452 1.00 0.00 H ATOM 1119 1HE LYS A 78153.401 -8.283 7.086 1.00 0.00 H ATOM 1120 2HE LYS A 78154.283 -9.339 8.188 1.00 0.00 H ATOM 1121 1HZ LYS A 78152.591 -8.817 9.553 1.00 0.00 H ATOM 1122 2HZ LYS A 78152.225 -7.371 8.757 1.00 0.00 H ATOM 1123 3HZ LYS A 78153.505 -7.426 9.860 1.00 0.00 H ATOM 1124 N ALA A 79155.202 -3.543 3.101 1.00 0.00 N

ATOM 1125 CA ALA A 79154.749 -2.238 2.635 1.00 0.00 C ATOM 1126 C ALA A 79154.591 -2.223 1.118 1.00 0.00 C ATOM 1127 O ALAA 79155.576 -2.254 0.381 1.00 0.00 O ATOM 1128 CB ALA A 79155.718 -1.153 3.077 1.00 0.00 C ATOM 1129 H ALAA 79155.872 -4.031 2.578 1.00 0.00 H ATOM 1130 HA ALAA 79153.789 -2.038 3.088 1.00 0.00 H ATOM 1131 1HB ALAA 79155.189 -0.216 3.177 1.00 0.00 H ATOM 1132 2HB ALA A 79156.501 -1.048 2.341 1.00 0.00 H ATOM 1133 3HB ALAA 79156.152 -1.425 4.029 1.00 0.00 H ATOM 1134 N LEUA 80153.345 -2.174 0.658 1.00 0.00 N ATOM 1135 CA LEU A 80153.058 -2.154 -0.771 1.00 0.00 C ATOM 1136 C LEU A 80152.216 -0.937 -1.140 1.00 0.00 C ATOM 1137 O LEUA 80151.022 -0.882 -0.847 1.00 0.00 O ATOM 1138 CB LEU A 80152.330 -3.434 -1.184 1.00 0.00 C ATOM 1139 CG LEU A 80151.917 -3.501 -2.655 1.00 0.00 C ATOM 1140 CD1 LEU A 80153.133 -3.730 -3.540 1.00 0.00 C ATOM 1141 CD2 LEU A 80150.885 -4.597 -2.871 1.00 0.00 C ATOM 1142 H LEUA 80152.600 -2.151 1.295 1.00 0.00 H ATOM 1143 HA LEU A 80153.998 -2.100 -1.298 1.00 0.00 H ATOM 1144 1HB LEU A 80152.976 -4.275 -0.975 1.00 0.00 H ATOM 1145 2HB LEU A 80151.439 -3.528 -0.580 1.00 0.00 H ATOM 1146 HG LEU A 80151.471 -2.559 -2.939 1.00 0.00 H ATOM 1147 1HD1 LEU A 80153.887 -4.268 -2.984 1.00 0.00 H ATOM 1148 2HD1 LEU A 80153.531 -2.777 -3.858 1.00 0.00 H ATOM 1149 3HD1 LEU A 80152.845 -4.307 -4.407 1.00 0.00 H ATOM 1150 1HD2 LEU A 80149.893 -4.181 -2.770 1.00 0.00 H ATOM 1151 2HD2 LEU A 80151.027 -5.374 -2.134 1.00 0.00 H ATOM 1152 3HD2 LEU A 80151.002 -5.012 -3.860 1.00 0.00 H ATOM 1153 N PHE A 81152.848 0.039 -1.786 1.00 0.00 N ATOM 1154 CA PHE A 81152.157 1.256 -2.195 1.00 0.00 C ATOM 1155 C PHE A 81151.307 1.009 -3.437 1.00 0.00 C

ATOM 1156 O PHE A 81151.705 0.267 -4.335 1.00 0.00 O ATOM 1157 CB PHE A 81153.167 2.373 -2.469 1.00 0.00 C ATOM 1158 CG PHE A 81153.932 2.803 -1.249 1.00 0.00 C ATOM 1159 CD1 PHE A 81153.577 3.955 -0.564 1.00 0.00 C ATOM 1160 CD2 PHE A 81155.004 2.057 -0.788 1.00 0.00 C ATOM 1161 CE1 PHE A 81154.278 4.354 0.558 1.00 0.00 C ATOM 1162 CE2 PHE A 81155.708 2.451 0.334 1.00 0.00 C ATOM 1163 CZ PHE A 81155.345 3.600 1.008 1.00 0.00 C ATOM 1164 H PHE A 81153.800 -0.062 -1.991 1.00 0.00 H ATOM 1165 HA PHE A 81151.511 1.559 -1.385 1.00 0.00 H ATOM 1166 1HB PHE A 81153.881 2.030 -3.203 1.00 0.00 H ATOM 1167 2HB PHE A 81152.644 3.235 -2.856 1.00 0.00 H ATOM 1168 HD1 PHE A 81152.742 4.544 -0.915 1.00 0.00 H ATOM 1169 HD2 PHE A 81155.289 1.158 -1.315 1.00 0.00 H ATOM 1170 HE1 PHE A 81153.992 5.253 1.082 1.00 0.00 H ATOM 1171 HE2 PHE A 81156.543 1.860 0.683 1.00 0.00 H ATOM 1172 HZ PHE A 81155.895 3.910 1.884 1.00 0.00 H ATOM 1173 N VALA 82150.136 1.635 -3.480 1.00 0.00 N ATOM 1174 CA VALA 82149.229 1.481 -4.612 1.00 0.00 C ATOM 1175 C VALA 82148.290 2.677 -4.731 1.00 0.00 C ATOM 1176 O VAL A 82148.185 3.490 -3.813 1.00 0.00 O ATOM 1177 CB VALA 82148.392 0.195 -4.492 1.00 0.00 C ATOM 1178 CG1 VAL A 82149.267 -1.034 -4.677 1.00 0.00 C ATOM 1179 CG2 VAL A 82147.673 0.150 -3.151 1.00 0.00 C ATOM 1180 H VALA 82149.874 2.213 -2.734 1.00 0.00 H ATOM 1181 HA VALA 82149.826 1.414 -5.510 1.00 0.00 H ATOM 1182 HB VALA 82147.648 0.200 -5.274 1.00 0.00 H ATOM 1183 1HG1 VAL A 82149.980 -1.095 -3.866 1.00 0.00 H ATOM 1184 2HG1 VAL A 82149.796 -0.961 -5.616 1.00 0.00 H ATOM 1185 3HG1 VAL A 82148.650 -1.920 -4.680 1.00 0.00 H ATOM 1186 1HG2 VAL A 82146.739 -0.382 -3.261 1.00 0.00 H

ATOM 1187 2HG2 VAL A 82147.476 1.157 -2.815 1.00 0.00 H ATOM 1188 3HG2 VAL A 82148.293 -0.357 -2.428 1.00 0.00 H ATOM 1189 N LYS A 83147.610 2.775 -5.868 1.00 0.00 N ATOM 1190 CA LYS A 83146.677 3.871 -6.108 1.00 0.00 C ATOM 1191 C LYS A 83145.454 3.754 -5.206 1.00 0.00 C ATOM 1192 O LYS A 83144.760 2.738 -5.212 1.00 0.00 O ATOM 1193 CB LYS A 83146.244 3.888 -7.574 1.00 0.00 C ATOM 1194 CG LYS A 83147.383 4.164 -8.542 1.00 0.00 C ATOM 1195 CD LYS A 83147.037 3.716 -9.953 1.00 0.00 C ATOM 1196 CE LYS A 83147.527 4.712 -10.991 1.00 0.00 C ATOM 1197 NZ LYS A 83147.970 4.039 -12.243 1.00 0.00 N ATOM 1198 H LYS A 83147.736 2.095 -6.562 1.00 0.00 H ATOM 1199 HA LYS A 83147.188 4.796 -5.882 1.00 0.00 H ATOM 1200 1HB LYS A 83145.815 2.929 -7.822 1.00 0.00 H ATOM 1201 2HB LYS A 83145.494 4.653 -7.708 1.00 0.00 H ATOM 1202 1HG LYS A 83147.585 5.225 -8.552 1.00 0.00 H ATOM 1203 2HG LYS A 83148.262 3.631 -8.210 1.00 0.00 H ATOM 1204 1HD LYS A 83147.501 2.760 -10.141 1.00 0.00 H ATOM 1205 2HD LYS A 83145.964 3.620 -10.037 1.00 0.00 H ATOM 1206 1HE LYS A 83146.723 5.394 -11.225 1.00 0.00 H ATOM 1207 2HE LYS A 83148.356 5.266 -10.576 1.00 0.00 H ATOM 1208 1HZ LYS A 83147.466 3.137 -12.361 1.00 0.00 H ATOM 1209 2HZ LYS A 83148.992 3.849 -12.204 1.00 0.00 H ATOM 1210 3HZ LYS A 83147.773 4.646 -13.064 1.00 0.00 H ATOM 1211 N LEUA 84145.197 4.803 -4.432 1.00 0.00 N ATOM 1212 CA LEU A 84144.059 4.823 -3.523 1.00 0.00 C ATOM 1213 C LEUA 84142.750 4.654 -4.288 1.00 0.00 C ATOM 1214 O LEU A 84141.796 4.062 -3.782 1.00 0.00 O ATOM 1215 CB LEU A 84144.039 6.133 -2.733 1.00 0.00 C ATOM 1216 CG LEU A 84142.825 6.326 -1.822 1.00 0.00 C ATOM 1217 CD1 LEU A 84142.924 5.419 -0.605 1.00 0.00 C

ATOM 1218 CD2 LEU A 84142.705 7.781 -1.396 1.00 0.00 C ATOM 1219 H LEUA 84145.789 5.582 -4.474 1.00 0.00 H ATOM 1220 HA LEU A 84144.169 3.999 -2.834 1.00 0.00 H ATOM 1221 1HB LEU A 84144.931 6.175 -2.125 1.00 0.00 H ATOM 1222 2HB LEU A 84144.066 6.952 -3.437 1.00 0.00 H ATOM 1223 HG LEU A 84141.930 6.059 -2.365 1.00 0.00 H ATOM 1224 1HD1 LEU A 84141.946 5.308 -0.159 1.00 0.00 H ATOM 1225 2HD1 LEU A 84143.600 5.855 0.115 1.00 0.00 H ATOM 1226 3HD1 LEU A 84143.294 4.450 -0.906 1.00 0.00 H ATOM 1227 1HD2 LEU A 84143.646 8.115 -0.986 1.00 0.00 H ATOM 1228 2HD2 LEU A 84141.931 7.874 -0.648 1.00 0.00 H ATOM 1229 3HD2 LEU A 84142.451 8.386 -2.254 1.00 0.00 H ATOM 1230 N LYS A 85142.712 5.177 -5.508 1.00 0.00 N ATOM 1231 CA LYS A 85141.521 5.083 -6.343 1.00 0.00 C ATOM 1232 C LYS A 85141.210 3.630 -6.689 1.00 0.00 C ATOM 1233 O LYS A 85140.057 3.274 -6.936 1.00 0.00 O ATOM 1234 CB LYS A 85141.707 5.896 -7.627 1.00 0.00 C ATOM 1235 CG LYS A 85143.008 5.597 -8.352 1.00 0.00 C ATOM 1236 CD LYS A 85142,945 6.026 -9.810 1.00 0.00 C ATOM 1237 CE LYS A 85142.666 4.847 -10.728 1.00 0.00 C ATOM 1238 NZ LYS A 85143.868 4.463 -11.521 1.00 0.00 N ATOM 1239 H LYS A 85143.505 5.637 -5.856 1.00 0.00 H ATOM 1240 HA LYS A 85140.693 5.494 -5.786 1.00 0.00 H ATOM 1241 1HB LYS A 85140.888 5.681 -8.297 1.00 0.00 H ATOM 1242 2HB LYS A 85141.691 6.947 -7.379 1.00 0.00 H ATOM 1243 1HG LYS A 85143.811 6.131 -7.866 1.00 0.00 H ATOM 1244 2HG LYS A 85143.200 4.535 -8.307 1.00 0.00 H ATOM 1245 1HD LYS A 85142.156 6.754 -9.927 1.00 0.00 H ATOM 1246 2HD LYS A 85143.890 6.470 -10.086 1.00 0.00 H ATOM 1247 1HE LYS A 85142.358 4.003 -10.129 1.00 0.00 H ATOM 1248 2HE LYS A 85141.869 5.116 -11.406 1.00 0.00 H

ATOM 1249 1HZ LYS A 85143.929 3.427 -11.599 1.00 0.00 H ATOM 1250 2HZ LYS A 85144.729 4.815 -11.058 1.00 0.00 H ATOM 1251 3HZ LYS A 85143.810 4.869 -12.477 1.00 0.00 H ATOM 1252 N SER A 86142.243 2.794 -6.705 1.00 0.00 N ATOM 1253 CA SER A 86142.077 1.380 -7.019 1.00 0.00 C ATOM 1254 C SER A 86142.051 0.539 -5.747 1.00 0.00 C ATOM 1255 O SER A 86142.486 -0.613 -5.743 1.00 0.00 O ATOM 1256 CB SER A 86143.205 0.904 -7.936 1.00 0.00 C ATOM 1257 OG SER A 86143.371 1.779 -9.038 1.00 0.00 O ATOM 1258 H SER A 86143.139 3.136 -6.500 1.00 0.00 H ATOM 1259 HA SER A 86141.134 1.264 -7.533 1.00 0.00 H ATOM 1260 1HB SER A 86144.128 0.869 -7.378 1.00 0.00 H ATOM 1261 2HB SER A 86142.972 -0.083 -8.308 1.00 0.00 H ATOM 1262 HG SER A 86142.512 1.998 -9.406 1.00 0.00 H ATOM 1263 N CYS A 87141.537 1.122 -4.669 1.00 0.00 N ATOM 1264 CA CYS A 87141.454 0.427 -3.390 1.00 0.00 C ATOM 1265 C CYS A 87140.001 0.231 -2.970 1.00 0.00 C ATOM 1266 O CYS A 87139.186 1.148 -3.073 1.00 0.00 O ATOM 1267 CB CYS A 87142.207 1.208 -2.311 1.00 0.00 C ATOM 1268 SG CYS A 87144.005 1.180 -2.501 1.00 0.00 S ATOM 1269 H CYS A 87141.206 2.042 -4.735 1.00 0.00 H ATOM 1270 HA CYS A 87141.916 -0.542 -3.508 1.00 0.00 H ATOM 1271 1HB CYS A 87141.891 2.239 -2.337 1.00 0.00 H ATOM 1272 2HB CYS A 87141.972 0.788 -1.344 1.00 0.00 H ATOM 1273 HG CYS A 87144.394 1.095 -1.627 1.00 0.00 H ATOM 1274 N ARG A 88139.683 -0.971 -2.498 1.00 0.00 N ATOM 1275 CA ARG A 88138.328 -1.288 -2.063 1.00 0.00 C ATOM 1276 C ARG A 88138.292 -1.575 -0.563 1.00 0.00 C ATOM 1277 O ARG A 88139.234 -2.142 -0.010 1.00 0.00 O ATOM 1278 CB ARG A 88137.790 -2.492 -2.839 1.00 0.00 C ATOM 1279 CG ARG A 88136.954 -2.109 -4.051 1.00 0.00 C

ATOM 1280 CD ARG A 88135.509 -2.558 -3.902 1.00 0.00 C ATOM 1281 NE ARG A 88135.240 -3.791 -4.638 1.00 0.00 N ATOM 1282 CZ ARG A 88134.146 -4.531 -4.470 1.00 0.00 C ATOM 1283 NH1 ARG A 88133.219 -4.168 -3.594 1.00 0.00 N ATOM 1284 NH2 ARG A 88133.980 -5.638 -5.181 1.00 0.00 N ATOM 1285 H ARG A 88140.377 -1.660 -2.441 1.00 0.00 H ATOM 1286 HA ARG A 88137.706 -0.430 -2.269 1.00 0.00 H ATOM 1287 1HB ARG A 88138.623 -3.088 -3.178 1.00 0.00 H ATOM 1288 2HB ARG A 88137.176 -3.087 -2.178 1.00 0.00 H ATOM 1289 1HG ARG A 88136.976 -1.035 -4.167 1.00 0.00 H ATOM 1290 2HG ARG A 88137.378 -2.575 -4.929 1.00 0.00 H ATOM 1291 1HD ARG A 88135.304 -2.724 -2.854 1.00 0.00 H ATOM 1292 2HD ARG A 88134.862 -1.778 -4.275 1.00 0.00 H ATOM 1293 HE ARG A 88135.910 -4.082 -5.292 1.00 0.00 H ATOM 1294 1HH1 ARG A 88133.338 -3.334 -3.054 1.00 0.00 H ATOM 1295 2HH1 ARG A 88132.399 -4.728 -3.472 1.00 0.00 H ATOM 1296 1HH2 ARG A 88134.676 -5.917 -5.843 1.00 0.00 H ATOM 1297 2HH2 ARG A 88133.159 -6.194 -5.055 1.00 0.00 H ATOM 1298 N PRO A 89137.198 -1.187 0.118 1.00 0.00 N ATOM 1299 CA PRO A 89137.048 -1.408 1.560 1.00 0.00 C ATOM 1300 C PRO A 89137.285 -2.863 1.950 1.00 0.00 C ATOM 1301 O PRO A 89136.808 -3.781 1.282 1.00 0.00 O ATOM 1302 CB PRO A 89135.594 -1.013 1.832 1.00 0.00 C ATOM 1303 CG PRO A 89135.252 -0.054 0.744 1.00 0.00 C ATOM 1304 CD PRO A 89136.026 -0.505 -0.463 1.00 0.00 C ATOM 1305 HA PRO A 89137.710 -0.771 2.128 1.00 0.00 H ATOM 1306 1HB PRO A 89134.967 -1.892 1.797 1.00 0.00 H ATOM 1307 2HB PRO A 89135.520 -0.549 2.803 1.00 0.00 H ATOM 1308 1HG PRO A 89134.191 -0.090 0.545 1.00 0.00 H ATOM 1309 2HG PRO A 89135.548 0.945 1.028 1.00 0.00 H ATOM 1310 1HD PRO A 89135.436 -1.189 -1.056 1.00 0.00 H

ATOM 1311 2HD PRO A 89136.329 0.346 -1.055 1.00 0.00 H ATOM 1312 N ASPA 90138.026 -3.066 3.035 1.00 0.00 N ATOM 1313 CA ASP A 90138.326 -4.409 3.514 1.00 0.00 C ATOM 1314 C ASP A 90137.405 -4.795 4.667 1.00 0.00 C ATOM 1315 O ASP A 90137.387 -4.137 5.706 1.00 0.00 O ATOM 1316 CB ASP A 90139.786 -4.499 3.961 1.00 0.00 C ATOM 1317 CG ASP A 90140.288 -5.929 4.013 1.00 0.00 C ATOM 1318 OD1 ASP A 90139.463 -6.840 4.238 1.00 0.00 O ATOM 1319 OD2 ASP A 90141.506 -6.138 3.828 1.00 0.00 O ATOM 1320 H ASP A 90138.378 -2.294 3.525 1.00 0.00 H ATOM 1321 HA ASP A 90138.167 -5.097 2.696 1.00 0.00 H ATOM 1322 1HB ASP A 90140.403 -3.947 3.268 1.00 0.00 H ATOM 1323 2HB ASP A 90139.881 -4.067 4.946 1.00 0.00 H ATOM 1324 N SER A 91136.640 -5.865 4.475 1.00 0.00 N ATOM 1325 CA SER A 91135.716 -6.338 5.498 1.00 0.00 C ATOM 1326 C SER A 91136.321 -7.495 6.286 1.00 0.00 C ATOM 1327 O SER A 91135.606 -8.375 6.764 1.00 0.00 O ATOM 1328 CB SER A 91134.396 -6.776 4.860 1.00 0.00 C ATOM 1329 OG SER A 91133.310 -6.584 5.749 1.00 0.00 O ATOM 1330 H SER A 91136.699 -6.348 3.624 1.00 0.00 H ATOM 1331 HA SER A 91135.523 -5.519 6.175 1.00 0.00 H ATOM 1332 1HB SER A 91134.221 -6.196 3.966 1.00 0.00 H ATOM 1333 2HB SER A 91134.454 -7.824 4.603 1.00 0.00 H ATOM 1334 HG SER A 91133.107 -7.412 6.191 1.00 0.00 H ATOM 1335 N ARG A 92137.643 -7.487 6.418 1.00 0.00 N ATOM 1336 CA ARG A 92138.345 -8.536 7.149 1.00 0.00 C ATOM 1337 C ARG A 92137.999 -8.490 8.633 1.00 0.00 C ATOM 1338 O ARG A 92137.991 -9.519 9.310 1.00 0.00 O ATOM 1339 CB ARG A 92139.856 -8.395 6.960 1.00 0.00 C ATOM 1340 CG ARG A 92140.387 -9.117 5.733 1.00 0.00 C ATOM 1341 CD ARG A 92140.922 -10.495 6.085 1.00 0.00 C ATOM 1342 NE ARG A 92139.849 -11.470 6.267 1.00 0.00 N ATOM 1343 CZ ARG A 92140.030 -12.682 6.784 1.00 0.00 C ATOM 1344 NH1 ARG A 92141.238 -13.075 7.169 1.00 0.00 N ATOM 1345 NH2 ARG A 92138.999 -13.508 6.915 1.00 0.00 N ATOM 1346 H ARG A 92138.160 -6.758 6.014 1.00 0.00 H ATOM 1347 HA ARG A 92138.029 -9.488 6.747 1.00 0.00 H ATOM 1348 1HB ARG A 92140.099 -7.347 6.869 1.00 0.00 H ATOM 1349 2HB ARG A 92140.355 -8.796 7.831 1.00 0.00 H ATOM 1350 1HG ARG A 92139.586 -9.225 5.016 1.00 0.00 H ATOM 1351 2HG ARG A 92141.183 -8.530 5.299 1.00 0.00 H ATOM 1352 1HD ARG A 92141.568 -10.830 5.287 1.00 0.00 H ATOM 1353 2HD ARG A 92141.491 -10.423 7.001 1.00 0.00 H ATOM 1354 HE ARG A 92138.947 -11.206 5.990 1.00 0.00 H ATOM 1355 1HH1 ARG A 92142.019 -12.458 7.074 1.00 0.00 H ATOM 1356 2HH1 ARG A 92141.367 -13.988 7.557 1.00 0.00 H ATOM 1357 1HH2 ARG A 92138.087 -13.217 6.626 1.00 0.00 H ATOM 1358 2HH2 ARG A 92139.135 -14.418 7.303 1.00 0.00 H ATOM 1359 N PHE A 93137.713 -7.293 9.133 1.00 0.00 N ATOM 1360 CA PHE A 93137.366 -7.114 10.538 1.00 0.00 C ATOM 1361 C PHE A 93136.006 -6.439 10.683 1.00 0.00 C ATOM 1362 O PHE A 93135.761 -5.713 11.646 1.00 0.00 O ATOM 1363 CB PHE A 93138.437 -6.284 11.248 1.00 0.00 C ATOM 1364 CG PHE A 93139.732 -7.019 11.447 1.00 0.00 C ATOM 1365 CD1 PHE A 93140.508 -7.389 10.360 1.00 0.00 C ATOM 1366 CD2 PHE A 93140.173 -7.340 12.721 1.00 0.00 C ATOM 1367 CE1 PHE A 93141.701 -8.064 10.540 1.00 0.00 C ATOM 1368 CE2 PHE A 93141.365 -8.015 12.907 1.00 0.00 C ATOM 1369 CZ PHE A 93142.129 -8.378 11.815 1.00 0.00 C ATOM 1370 H PHE A 93137.736 -6.511 8.543 1.00 0.00 H ATOM 1371 HA PHE A 93137.320 -8.091 10.995 1.00 0.00 H ATOM 1372 1HB PHE A 93138.644 -5.400 10.663 1.00 0.00 H

ATOM 1373 2HB PHE A 93138.069 -5.989 12.219 1.00 0.00 H ATOM 1374 HD1 PHE A 93140.174 -7.143 9.362 1.00 0.00 H ATOM 1375 HD2 PHE A 93139.576 -7.057 13.575 1.00 0.00 H ATOM 1376 HE1 PHE A 93142.296 -8.347 9.684 1.00 0.00 H ATOM 1377 HE2 PHE A 93141.697 -8.260 13.905 1.00 0.00 H ATOM 1378 HZ PHE A 93143.060 -8.906 11.957 1.00 0.00 H ATOM 1379 N ALA A 94135.123 -6.684 9.719 1.00 0.00 N ATOM 1380 CA ALA A 94133.788 -6.099 9.741 1.00 0.00 C ATOM 1381 C ALA A 94132.772 -7.072 10.327 1.00 0.00 C ATOM 1382 O ALA A 94132.691 -8.228 9.909 1.00 0.00 O ATOM 1383 CB ALA A 94133.373 -5.682 8.337 1.00 0.00 C ATOM 1384 H ALAA 94135.376 -7.271 8.976 1.00 0.00 H ATOM 1385 HA ALA A 94133.822 -5.214 10.358 1.00 0.00 H ATOM 1386 1HB ALA A 94134.251 -5.568 7.721 1.00 0.00 H ATOM 1387 2HB ALA A 94132.841 -4.743 8.384 1.00 0.00 H ATOM 1388 3HB ALA A 94132.730 -6.439 7.913 1.00 0.00 H ATOM 1389 N SER A 95131.999 -6.600 11.299 1.00 0.00 N ATOM 1390 CA SER A 95130.987 -7.428 11.944 1.00 0.00 C ATOM 1391 C SER A 95129.662 -7.353 11.194 1.00 0.00 C ATOM 1392 O SER A 95129.017 -6.305 11.158 1.00 0.00 O ATOM 1393 CB SER A 95130.791 -6.992 13.397 1.00 0.00 C ATOM 1394 OG SER A 95130.890 -5.584 13.525 1.00 0.00 O ATOM 1395 H SER A 95132.110 -5.670 11.589 1.00 0.00 H ATOM 1396 HA SER A 95131.338 -8.450 11.928 1.00 0.00 H ATOM 1397 1HB SER A 95129.814 -7.304 13.735 1.00 0.00 H ATOM 1398 2HB SER A 95131.549 -7.453 14.013 1.00 0.00 H ATOM 1399 HG SER A 95130.226 -5.272 14.144 1.00 0.00 H ATOM 1400 N LEUA 96129.260 -8.471 10.598 1.00 0.00 N ATOM 1401 CA LEU A 96128.010 -8.531 9.849 1.00 0.00 C ATOM 1402 C LEU A 96127.168 -9.724 10.295 1.00 0.00 C ATOM 1403 O LEU A 96126.898 -10.636 9.512 1.00 0.00 O

ATOM 1404 CB LEU A 96128.294 -8.620 8.348 1.00 0.00 C ATOM 1405 CG LEU A 96128.449 -7.275 7.638 1.00 0.00 C ATOM 1406 CD1 LEU A 96129.872 -6.756 7.782 1.00 0.00 C ATOM 1407 CD2 LEU A 96128.074 -7.403 6.170 1.00 0.00 C ATOM 1408 H LEU A 96129.818 -9.273 10.663 1.00 0.00 H ATOM 1409 HA LEU A 96127.459 -7.624 10.049 1.00 0.00 H ATOM 1410 1HB LEU A 96129.204 -9.186 8.209 1.00 0.00 H ATOM 1411 2HB LEU A 96127.483 -9.158 7.881 1.00 0.00 H ATOM 1412 HG LEU A 96127.785 -6.556 8.093 1.00 0.00 H ATOM 1413 1HD1 LEU A 96130.148 -6.210 6.893 1.00 0.00 H ATOM 1414 2HD1 LEU A 96130.546 -7.589 7.917 1.00 0.00 H ATOM 1415 3HD1 LEU A 96129.932 -6.102 8.639 1.00 0.00 H ATOM 1416 1HD2 LEU A 96128.564 -6.626 5.603 1.00 0.00 H ATOM 1417 2HD2 LEU A 96127.003 -7.305 6.063 1.00 0.00 H ATOM 1418 3HD2 LEU A 96128.385 -8.368 5.800 1.00 0.00 H ATOM 1419 N GLN A 97126.757 -9.711 11.559 1.00 0.00 N ATOM 1420 CA GLN A 97125.947 -10.790 12.110 1.00 0.00 C ATOM 1421 C GLN A 97124.516 -10.728 11.576 1.00 0.00 C ATOM 1422 O GLN A 97124.045 -11.665 10.932 1.00 0.00 O ATOM 1423 CB GLN A 97125.941 -10.721 13.640 1.00 0.00 C ATOM 1424 CG GLN A 97126.526 -11.955 14.306 1.00 0.00 C ATOM 1425 CD GLN A 97127.328 -11.623 15.549 1.00 0.00 C ATOM 1426 OE1 GLN A 97128.215 -10.768 15.519 1.00 0.00 O ATOM 1427 NE2 GLN A 97127.020 -12.297 16.650 1.00 0.00 N ATOM 1428 H GLN A 97127.004 -8.958 12.134 1.00 0.00 H ATOM 1429 HA GLN A 97126.390 -11.726 11.804 1.00 0.00 H ATOM 1430 1HB GLN A 97126.519 -9.863 13.952 1.00 0.00 H ATOM 1431 2HB GLN A 97124.924 -10.602 13.982 1.00 0.00 H ATOM 1432 1HG GLN A 97125.719 -12.616 14.585 1.00 0.00 H ATOM 1433 2HG GLN A 97127.173 -12.457 13.601 1.00 0.00 H ATOM 1434 1HE2 GLN A 97126.303 -12.963 16.600 1.00 0.00 H

ATOM 1435 2HE2 GLN A 97127.523 -12.101 17.468 1.00 0.00 H ATOM 1436 N PRO A 98123.805 -9.618 11.839 1.00 0.00 N ATOM 1437 CA PRO A 98122.423 -9.441 11.383 1.00 0.00 C ATOM 1438 C PRO A 98122.336 -9.185 9.882 1.00 0.00 C ATOM 1439 O PRO A 98121.504 -9.772 9.190 1.00 0.00 O ATOM 1440 CB PRO A 98121.948 -8.215 12.163 1.00 0.00 C ATOM 1441 CG PRO A 98123.189 -7.437 12.434 1.00 0.00 C ATOM 1442 CD PRO A 98124.289 -8.450 12.603 1.00 0.00 C ATOM 1443 HA PRO A 98121.811 -10.293 11.637 1.00 0.00 H ATOM 1444 1HB PRO A 98121.251 -7.650 11.562 1.00 0.00 H ATOM 1445 2HB PRO A 98121.472 -8.530 13.079 1.00 0.00 H ATOM 1446 1HG PRO A 98123.404 -6.786 11.600 1.00 0.00 H ATOM 1447 2HG PRO A 98123.070 -6.861 13.341 1.00 0.00 H ATOM 1448 1HD PRO A 98125.213 -8.076 12.188 1.00 0.00 H ATOM 1449 2HD PRO A 98124.416 -8.700 13.646 1.00 0.00 H ATOM 1450 N SER A 99123.200 -8.306 9.385 1.00 0.00 N ATOM 1451 CA SER A 99123.219 -7.974 7.965 1.00 0.00 C ATOM 1452 C SER A 99121.874 -7.407 7.521 1.00 0.00 C ATOM 1453 O SER A 99121.020 -7.091 8.348 1.00 0.00 O ATOM 1454 CB SER A 99123.566 -9.211 7.134 1.00 0.00 C ATOM 1455 OG SER A 99124.331 -8.862 5.994 1.00 0.00 O ATOM 1456 H SER A 99123.840 -7.871 9.986 1.00 0.00 H ATOM 1457 HA SER A 99123.981 -7.223 7.811 1.00 0.00 H ATOM 1458 1HB SER A 99124.136 -9.899 7.738 1.00 0.00 H ATOM 1459 2HB SER A 99122.654 -9.689 6.808 1.00 0.00 H ATOM 1460 HG SER A 99124.982 -9.547 5.823 1.00 0.00 H ATOM 1461 N GLY A 100121.693 -7.282 6.210 1.00 0.00 N ATOM 1462 CA GLY A 100120.450 -6.753 5.680 1.00 0.00 C ATOM 1463 C GLY A 100119.356 -7.803 5.611 1.00 0.00 C ATOM 1464 O GLY A 100119.639 -8.982 5.399 1.00 0.00 O ATOM 1465 H GLY A 100122.411 -7.550 5.597 1.00 0.00 H

ATOM 1466 1HA GLY A 100120.118 -5.944 6.312 1.00 0.00 H ATOM 1467 2HA GLY A 100120.628 -6.370 4.686 1.00 0.00 H ATOM 1468 N PRO A 101118.085 -7.404 5.789 1.00 0.00 N ATOM 1469 CA PRO A 101116.952 -8.333 5.743 1.00 0.00 C ATOM 1470 C PRO A 101116.660 -8.821 4.328 1.00 0.00 C ATOM 1471 O PRO A 101116.427 -8.023 3.421 1.00 0.00 O ATOM 1472 CB PRO A 101115.786 -7.494 6.269 1.00 0.00 C ATOM 1473 CG PRO A 101116.154 -6.088 5.942 1.00 0.00 C ATOM 1474 CD PRO A 101117.653 -6.016 6.049 1.00 0.00 C ATOM 1475 HA PRO A 101117.110 -9.182 6.391 1.00 0.00 H ATOM 1476 1HB PRO A 101114.873 -7.791 5.773 1.00 0.00 H ATOM 1477 2HB PRO A 101115.686 -7.638 7.335 1.00 0.00 H ATOM 1478 1HG PRO A 101115.838 -5.850 4.937 1.00 0.00 H ATOM 1479 2HG PRO A 101115.696 -5.414 6.650 1.00 0.00 H ATOM 1480 1HD PRO A 101118.052 -5.343 5.304 1.00 0.00 H ATOM 1481 2HD PRO A 101117.947 -5.701 7.039 1.00 0.00 H ATOM 1482 N SER A 102116.674 -10.138 4.148 1.00 0.00 N ATOM 1483 CA SER A 102116.412 -10.733 2.842 1.00 0.00 C ATOM 1484 C SER A 102116.109 -12.222 2.974 1.00 0.00 C ATOM 1485 O SER A 102114.991 -12.664 2.712 1.00 0.00 O ATOM 1486 CB SER A 102117.608 -10.524 1.913 1.00 0.00 C ATOM 1487 OG SER A 102118.116 -9.206 2.023 1.00 0.00 O ATOM 1488 H SER A 102116.867 -10.723 4.910 1.00 0.00 H ATOM 1489 HA SER A 102115.549 -10.239 2.421 1.00 0.00 H ATOM 1490 1HB SER A 102118.391 -11.220 2.174 1.00 0.00 H ATOM 1491 2HB SER A 102117.301 -10.695 0.891 1.00 0.00 H ATOM 1492 HG SER A 102117.394 -8.577 1.950 1.00 0.00 H ATOM 1493 N SER A 103117.113 -12.991 3.383 1.00 0.00 N ATOM 1494 CA SER A 103116.954 -14.431 3.549 1.00 0.00 C ATOM 1495 C SER A 103116.257 -14.753 4.867 1.00 0.00 C ATOM 1496 O SER A 103115.461 -15.689 4.948 1.00 0.00 O

ATOM 1497 CB SER A 103118.316 -15.125 3.496 1.00 0.00 C ATOM 1498 OG SER A 103119.347 -14.261 3.943 1.00 0.00 O ATOM 1499 H SER A 103117.982 -12.580 3.576 1.00 0.00 H ATOM 1500 HA SER A 103116.344 -14.793 2.735 1.00 0.00 H ATOM 1501 1HB SER A 103118.297 -15.999 4.129 1.00 0.00 H ATOM 1502 2HB SER A 103118.528 -15.422 2.480 1.00 0.00 H ATOM 1503 HG SER A 103119.084 -13.850 4.770 1.00 0.00 H ATOM 1504 N GLY A 104116.563 -13.971 5.898 1.00 0.00 N ATOM 1505 CA GLY A 104115.957 -14.190 7.198 1.00 0.00 C ATOM 1506 C GLY A 104116.797 -13.632 8.330 1.00 0.00 C ATOM 1507 O GLY A 104116.544 -12.483 8.749 1.00 0.00 O ATOM 1508 OXT GLY A 104117.710 -14.346 8.800 1.00 0.00 O ATOM 1509 H GLY A 104117.204 -13.241 5.775 1.00 0.00 H ATOM 1510 1HA GLY A 104114.988 -13.713 7.216 1.00 0.00 H ATOM 1511 2HA GLY A 104115.828 -15.251 7.349 1.00 0.00 H TER 1512 GLY A 104 **ENDMDL**

Three-Dimensional Structure Coordinate Table 4

ATOM 1 N GLY A 1121.720 20.634 -14.920 1.00 0.00 N
ATOM 2 CA GLY A 1122.817 20.620 -15.926 1.00 0.00 C
ATOM 3 C GLY A 1124.008 19.798 -15.473 1.00 0.00 C
ATOM 4 O GLY A 1124.328 18.773 -16.074 1.00 0.00 O
ATOM 5 1H GLY A 1121.802 19.811 -14.289 1.00 0.00 H
ATOM 6 2H GLY A 1120.797 20.600 -15.398 1.00 0.00 H
ATOM 7 3H GLY A 1121.770 21.502 -14.350 1.00 0.00 H
ATOM 8 1HA GLY A 1122.439 20.205 -16.849 1.00 0.00 H
ATOM 9 2HA GLY A 1123.140 21.634 -16.106 1.00 0.00 H
ATOM 10 N SER A 2124.667 20.251 -14.411 1.00 0.00 N
ATOM11 CA SER A 2125.830 19.552 -13.878 1.00 0.00 C

ATOM13 O SER A 2126.259 18.661 -11.690 1.00 0.00 O ATOM14 CB SER A 2126.948 20.547 -13.561 1.00 0.00 C ATOM15 OG SER A 2126.520 21.513 -12.617 1.00 0.00 O ATOM16 H SER A 2124.363 21.075 -13.976 1.00 0.00 H ATOM17 HA SER A 2126.177 18.862 -14.633 1.00 0.00 H ATOM18 1HB SER A 2127.796 20.015 -13.156 1.00 0.00 H ATOM19 2HB SER A 2127.243 21.054 -14.469 1.00 0.00 H ATOM20 HG SER A 2126.598 22.391 -12.998 1.00 0.00 H ATOM21 N SER A 3124.255 18.213 -12.610 1.00 0.00 N ATOM22 CA SER A 3123.782 17.436 -11.469 1.00 0.00 C ATOM23 C SER A 3123.253 16.078 -11.920 1.00 0.00 C ATOM24 O SER A 3123.214 15.780 -13.113 1.00 0.00 O ATOM25 CB SER A 3122.690 18.201 -10.721 1.00 0.00 C ATOM26 OG SER A 3122.954 19.592 -10.713 1.00 0.00 O ATOM27 H SER A 3123.666 18.332 -13.384 1.00 0.00 H ATOM28 HA SER A 3124.619 17.280 -10.805 1.00 0.00 H ATOM29 1HB SER A 3121.739 18.031 -11.206 1.00 0.00 H ATOM30 2HB SER A 3122.641 17.848 -9.701 1.00 0.00 H ATOM31 HG SER A 3123.781 19.758 -10.252 1.00 0.00 H ATOM32 N GLY A 4122.847 15.258 -10.956 1.00 0.00 N ATOM33 CA GLY A 4122.325 13.942 -11.272 1.00 0.00 C ATOM34 C GLY A 4121.131 13.570 -10.416 1.00 0.00 C ATOM35 O GLY A 4120.014 13.442 -10.917 1.00 0.00 O ATOM36 H GLY A 4122.901 15.549 -10.021 1.00 0.00 H ATOM37 1HA GLY A 4122.029 13.925 -12.310 1.00 0.00 H ATOM38 2HA GLY A 4123.105 13.211 -11.120 1.00 0.00 H ATOM39 N SER A 5121.366 13.394 -9.120 1.00 0.00 N ATOM40 CA SER A 5120.300 13.034 -8.191 1.00 0.00 C ATOM41 C SER A 5120.725 13.292 -6.750 1.00 0.00 C ATOM42 O SER A 5121.804 13.829 -6.496 1.00 0.00 O ATOM43 CB SER A 5119.918 11.564 -8.367 1.00 0.00 C

ATOM44 OG SER A 5118.602 11.319 -7.902 1.00 0.00 O ATOM45 H SER A 5122.278 13.510 -8.780 1.00 0.00 H ATOM46 HA SER A 5119.443 13.650 -8.417 1.00 0.00 H ATOM47 1HB SER A 5119,969 11.303 -9.414 1.00 0.00 H ATOM48 2HB SER A 5120.605 10.946 -7.809 1.00 0.00 H ATOM49 HG SER A 5117.985 11.880 -8.377 1.00 0.00 H ATOM50 N SER A 6119.871 12.904 -5.808 1.00 0.00 N ATOM51 CA SER A 6120.158 13.094 -4.391 1.00 0.00 C ATOM52 C SER A 6120.904 11.891 -3.822 1.00 0.00 C ATOM53 O SER A 6120.766 10.772 -4.314 1.00 0.00 O ATOM54 CB SER A 6118.860 13.318 -3.612 1.00 0.00 C ATOM55 OG SER A 6118.541 14.697 -3.538 1.00 0.00 O ATOM56 H SER A 6119.027 12.481 -6.073 1.00 0.00 H ATOM57 HA SER A 6120.782 13.969 -4.293 1.00 0.00 H ATOM58 1HB SER A 6118.052 12.801 -4.106 1.00 0.00 H ATOM59 2HB SER A 6118.975 12.933 -2.609 1.00 0.00 H ATOM60 HG SER A 6118.107 14.880 -2.702 1.00 0.00 H ATOM61 N GLY A 7121.697 12.132 -2.782 1.00 0.00 N ATOM62 CA GLY A 7122.455 11.059 -2.163 1.00 0.00 C ATOM63 C GLY A 7123.939 11.360 -2.100 1.00 0.00 C ATOM64 O GLY A 7124.349 12.392 -1.568 1.00 0.00 O ATOM65 H GLY A 7121.768 13.044 -2.433 1.00 0.00 H ATOM66 1HA GLY A 7122.086 10.908 -1.159 1.00 0.00 H ATOM67 2HA GLY A 7122.306 10.153 -2.730 1.00 0.00 H ATOM68 N LEUA 8124.747 10.455 -2.645 1.00 0.00 N ATOM69 CA LEU A 8126.195 10.628 -2.648 1.00 0.00 C ATOM70 C LEU A 8126.735 10.727 -1.225 1.00 0.00 C ATOM71 O LEUA 8126.956 11.822 -0.708 1.00 0.00 O ATOM72 CB LEU A 8126.578 11.881 -3.439 1.00 0.00 C ATOM73 CG LEUA 8126.391 11.771 -4.954 1.00 0.00 C ATOM74 CD1 LEU A 8125.132 12.503 -5.392 1.00 0.00 C ATOM75 CD2 LEU A 8127.609 12.320 -5.684 1.00 0.00 C ATOM76 H LEUA 8124.360 9.653 -3.053 1.00 0.00 H ATOM77 HA LEU A 8126.631 9.764 -3.127 1.00 0.00 H ATOM78 1HB LEU A 8125.979 12.704 -3.080 1.00 0.00 H ATOM79 2HB LEU A 8127.617 12.101 -3.241 1.00 0.00 H ATOM80 HG LEU A 8126.281 10.731 -5.222 1.00 0.00 H ATOM81 1HD1 LEU A 8125.389 13.502 -5.716 1.00 0.00 H ATOM82 2HD1 LEU A 8124.442 12.560 -4.564 1.00 0.00 H ATOM83 3HD1 LEU A 8124.669 11.968 -6.208 1.00 0.00 H ATOM84 1HD2 LEU A 8127.471 12.206 -6.749 1.00 0.00 H ATOM85 2HD2 LEU A 8128.489 11.776 -5.375 1.00 0.00 H ATOM86 3HD2 LEU A 8127.731 13.366 -5.447 1.00 0.00 H ATOM87 N ALAA 9126.946 9.575 -0.597 1.00 0.00 N ATOM88 CA ALA A 9127.461 9.530 0.766 1.00 0.00 C ATOM89 C ALA A 9128.987 9.538 0.777 1.00 0.00 C ATOM90 O ALAA 9129.620 8.618 1.295 1.00 0.00 O ATOM91 CB ALA A 9126.930 8.302 1.490 1.00 0.00 C ATOM92 H ALAA 9126.752 8.734 -1.062 1.00 0.00 H ATOM93 HA ALA A 9127.103 10.408 1.285 1.00 0.00 H ATOM94 1HB ALA A 9126.984 7.446 0.834 1.00 0.00 H ATOM95 2HB ALA A 9125.902 8.470 1.778 1.00 0.00 H ATOM96 3HB ALA A 9127.525 8.119 2.372 1.00 0.00 H ATOM97 N MET A 10129.571 10.584 0.201 1.00 0.00 N ATOM98 CA MET A 10131.023 10.712 0.145 1.00 0.00 C ATOM99 C MET A 10131.429 12.104 -0.337 1.00 0.00 C ATOM 100 O MET A 10132.025 12.252 -1.405 1.00 0.00 O 101 CB META 10131.614 9.645 -0.779 1.00 0.00 C ATOM 102 CG MET A 10130.848 9.478 -2.083 1.00 0.00 C ATOM ATOM 103 SD MET A 10131.914 9.566 -3.535 1.00 0.00 S ATOM 104 CE MET A 10131.189 10.954 -4.404 1.00 0.00 C ATOM 105 H MET A 10129.013 11.286 -0.194 1.00 0.00 H

ATOM 106 HA META 10131.407 10.564 1.143 1.00 0.00 H **ATOM** 107 1HB META 10132.633 9.913 -1.014 1.00 0.00 H ATOM 108 2HB META 10131.611 8.697 -0.261 1.00 0.00 H **ATOM** 109 1HG META 10130.356 8.517 -2.075 1.00 0.00 H **ATOM** 110 2HG META 10130.106 10.259 -2.151 1.00 0.00 H **ATOM** 111 1HE META 10130.247 10.653 -4.838 1.00 0.00 H **ATOM** 112 2HE MET A 10131.859 11.279 -5.186 1.00 0.00 H ATOM 113 3HE META 10131.023 11.765 -3.711 1.00 0.00 H **ATOM** 114 N PRO A 11131.111 13.149 0.447 1.00 0.00 N ATOM 115 CA PRO A 11131.448 14.531 0.093 1.00 0.00 C **ATOM** 116 C PROA 11132.950 14.732 -0.102 1.00 0.00 C **ATOM** 117 O PROA 11133.376 15.329 -1.090 1.00 0.00 O **ATOM** 118 CB PRO A 11130.946 15.355 1.283 1.00 0.00 C **ATOM** 119 CG PRO A 11129.966 14.479 1.987 1.00 0.00 C **ATOM** 120 CD PRO A 11130.402 13.063 1.735 1.00 0.00 C **ATOM** 121 HA PRO A 11130.931 14.840 -0.803 1.00 0.00 H ATOM 122 1HB PRO A 11131.778 15.610 1.923 1.00 0.00 H **ATOM** 123 2HB PRO A 11130.476 16.258 0.923 1.00 0.00 H ATOM 124 1HG PRO A 11129.982 14.690 3.045 1.00 0.00 H **ATOM** 125 2HG PRO A 11128.975 14.641 1.587 1.00 0.00 H ATOM 126 1HD PRO A 11131.065 12.727 2.519 1.00 0.00 H **ATOM** 127 2HD PRO A 11129.544 12.412 1.659 1.00 0.00 H ATOM 128 N PRO A 12133.779 14.235 0.835 1.00 0.00 N ATOM 129 CA PRO A 12135.238 14.369 0.742 1.00 0.00 C ATOM 130 C PRO A 12135.783 13.801 -0.562 1.00 0.00 C 131 O PROA 12136.871 14.169 -1.006 1.00 0.00 O ATOM ATOM 132 CB PRO A 12135.755 13.558 1.934 1.00 0.00 C 133 CG PRO A 12134.615 13.509 2.890 1.00 0.00 C ATOM ATOM 134 CD PRO A 12133.371 13.501 2.049 1.00 0.00 C ATOM 135 HA PRO A 12135.546 15.399 0.841 1.00 0.00 H ATOM 136 1HB PRO A 12136.037 12.568 1.604 1.00 0.00 H

ATOM 137 2HB PRO A 12136.611 14.055 2.366 1.00 0.00 H 138 1HG PRO A 12134.672 12.609 3.484 1.00 0.00 H ATOM ATOM 139 2HG PRO A 12134.632 14.382 3.526 1.00 0.00 H 140 1HD PRO A 12133.084 12.488 1.809 1.00 0.00 H ATOM **ATOM** 141 2HD PRO A 12132.570 14.012 2.558 1.00 0.00 H 142 N GLY A 13135.020 12.900 -1.175 1.00 0.00 N ATOM 143 CA GLY A 13135.443 12.293 -2.423 1.00 0.00 C **ATOM** 144 C GLY A 13135.739 10.814 -2.278 1.00 0.00 C ATOM 145 O GLY A 13135.196 10.149 -1.395 1.00 0.00 O **ATOM** 146 H GLY A 13134.162 12.644 -0.774 1.00 0.00 H ATOM 147 1HA GLY A 13134.662 12.423 -3.156 1.00 0.00 H **ATOM** 148 2HA GLY A 13136.335 12.795 -2.771 1.00 0.00 H ATOM 149 N ASNA 14136.601 10.296 -3.147 1.00 0.00 N **ATOM** 150 CA ASN A 14136.968 8.885 -3.112 1.00 0.00 C ATOM ATOM 151 C ASNA 14135.742 7.999 -3.313 1.00 0.00 C 152 O ASN A 14134.635 8.494 -3.530 1.00 0.00 O **ATOM** 153 CB ASN A 14137.644 8.545 -1.783 1.00 0.00 C ATOM 154 CG ASN A 14138.954 9.284 -1.595 1.00 0.00 C **ATOM** 155 OD1 ASN A 14139.305 10.161 -2.385 1.00 0.00 O **ATOM** 156 ND2 ASN A 14139.687 8.933 -0.545 1.00 0.00 N **ATOM** 157 H ASNA 14137.000 10.876 -3.828 1.00 0.00 H **ATOM** 158 HA ASN A 14137.664 8.704 -3.917 1.00 0.00 H **ATOM** 159 1HB ASN A 14136.983 8.810 -0.971 1.00 0.00 H **ATOM** 160 2HB ASN A 14137.842 7.484 -1.747 1.00 0.00 H **ATOM** 161 1HD2 ASN A 14139.345 8.227 0.043 1.00 0.00 H **ATOM** 162 2HD2 ASN A 14140.538 9.395 -0.399 1.00 0.00 H **ATOM** 163 N SER A 15135.948 6.689 -3.242 1.00 0.00 N ATOM 164 CA SER A 15134.858 5.734 -3.416 1.00 0.00 C ATOM 165 C SER A 15133.890 5.791 -2.239 1.00 0.00 C **ATOM** 166 O SER A 15132.711 6.101 -2.407 1.00 0.00 O ATOM 167 CB SER A 15135.414 4.317 -3.566 1.00 0.00 C ATOM

ATOM 168 OG SER A 15136.208 3.959 -2.448 1.00 0.00 O 169 H SER A 15136.852 6.355 -3.068 1.00 0.00 H ATOM **ATOM** 170 HA SER A 15134.326 5.999 -4.317 1.00 0.00 H 171 1HB SER A 15134.595 3.618 -3.647 1.00 0.00 H ATOM ATOM 172 2HB SER A 15136.023 4.263 -4.456 1.00 0.00 H 173 HG SER A 15137.082 3.698 -2.747 1.00 0.00 H ATOM **ATOM** 174 N HIS A 16134.398 5.491 -1.048 1.00 0.00 N **ATOM** 175 CA HIS A 16133.578 5.509 0.159 1.00 0.00 C **ATOM** 176 C HIS A 16134.260 6.307 1.267 1.00 0.00 C ATOM 177 O HIS A 16133.836 7.413 1.599 1.00 0.00 O 178 CB HIS A 16133.304 4.080 0.634 1.00 0.00 C **ATOM ATOM** 179 CG HIS A 16131.900 3.624 0.378 1.00 0.00 C 180 ND1 HIS A 16131.007 3.335 1.388 1.00 0.00 N **ATOM** 181 CD2 HIS A 16131.237 3.409 -0.782 1.00 0.00 C **ATOM** 182 CE1 HIS A 16129.855 2.961 0.860 1.00 0.00 C ATOM **ATOM** 183 NE2 HIS A 16129.968 2.997 -0.455 1.00 0.00 N 184 H HIS A 16135.345 5.253 -0.978 1.00 0.00 H ATOM **ATOM** 185 HA HIS A 16132.640 5.984 -0.086 1.00 0.00 H 186 1HB HIS A 16133.970 3.403 0.122 1.00 0.00 H ATOM **ATOM** 187 2HB HIS A 16133.485 4.019 1.698 1.00 0.00 H 188 HD1 HIS A 16131.190 3.395 2.350 1.00 0.00 H **ATOM** 189 HD2 HIS A 16131.632 3.536 -1.780 1.00 0.00 H ATOM 190 HE1 HIS A 16128.971 2.675 1.411 1.00 0.00 H ATOM 191 HE2 HIS A 16129.289 2.685 -1.088 1.00 0.00 H **ATOM** 192 N GLY A 17135.318 5.736 1.834 1.00 0.00 N **ATOM ATOM** 193 CA GLY A 17136.041 6.408 2.898 1.00 0.00 C 194 C GLYA 17137.368 5.742 3.205 1.00 0.00 C **ATOM** 195 O GLYA 17137.614 5.325 4.336 1.00 0.00 O ATOM 196 H GLYA 17135.609 4.853 1.527 1.00 0.00 H **ATOM** 197 1HA GLY A 17136.223 7.431 2.604 1.00 0.00 H **ATOM** 198 2HA GLY A 17135.433 6.403 3.791 1.00 0.00 H ATOM

199 N LEUA 18138.224 5.641 2.194 1.00 0.00 N **ATOM** 200 CA LEU A 18139.533 5.020 2.360 1.00 0.00 C **ATOM** 201 C LEUA 18140.585 6.058 2.735 1.00 0.00 C 202 O LEUA 18140.997 6.868 1.904 1.00 0.00 O ATOM **ATOM** 203 CB LEU A 18139.946 4.299 1.074 1.00 0.00 C 204 CG LEU A 18138.884 3.370 0.484 1.00 0.00 C **ATOM ATOM** 205 CD1 LEU A 18139.224 3.020 -0.957 1.00 0.00 C 206 CD2 LEU A 18138.754 2.110 1.325 1.00 0.00 C ATOM ATOM 207 H LEUA 18137.969 5.991 1.314 1.00 0.00 H ATOM 208 HA LEU A 18139.458 4.296 3.158 1.00 0.00 H 209 1HB LEU A 18140.195 5.046 0.333 1.00 0.00 H ATOM **ATOM** 210 2HB LEU A 18140.828 3.714 1.282 1.00 0.00 H 211 HG LEU A 18137.929 3.877 0.487 1.00 0.00 H **ATOM** 212 1HD1 LEU A 18140.293 3.082 -1.099 1.00 0.00 H ATOM 213 2HD1 LEU A 18138.731 3.712 -1.622 1.00 0.00 H ATOM 214 3HD1 LEU A 18138.890 2.015 -1.171 1.00 0.00 H ATOM 215 1HD2 LEU A 18139.718 1.634 1.411 1.00 0.00 H ATOM 216 2HD2 LEU A 18138.058 1.432 0.852 1.00 0.00 H **ATOM** 217 3HD2 LEU A 18138.390 2.369 2.308 1.00 0.00 H ATOM 218 N GLUA 19141.017 6.028 3.992 1.00 0.00 N 219 CA GLUA 19142.022 6.965 4.478 1.00 0.00 C ATOM 220 C GLUA 19143.071 6.248 5.321 1.00 0.00 C **ATOM** 221 O GLUA 19143.018 5.031 5.491 1.00 0.00 O ATOM 222 CB GLU A 19141.360 8.074 5.299 1.00 0.00 C **ATOM ATOM** 223 CG GLUA 19140.503 7.556 6.441 1.00 0.00 C 224 CD GLUA 19139.214 8.339 6.604 1.00 0.00 C **ATOM** 225 OE1 GLU A 19138.659 8.787 5.579 1.00 0.00 O **ATOM** 226 OE2 GLU A 19138.761 8.502 7.756 1.00 0.00 O **ATOM** 227 H GLU A 19140.651 5.358 4.607 1.00 0.00 H ATOM 228 HA GLU A 19142.506 7.405 3.619 1.00 0.00 H ATOM ATOM 229 1HB GLU A 19142.132 8.706 5.714 1.00 0.00 H

230 2HB GLU A 19140.735 8.664 4.646 1.00 0.00 H **ATOM ATOM** 231 1HG GLU A 19140.256 6.523 6.249 1.00 0.00 H **ATOM** 232 2HG GLUA 19141.068 7.626 7.359 1.00 0.00 H 233 N VALA 20144.023 7.011 5.846 1.00 0.00 N **ATOM ATOM** 234 CA VAL A 20145.085 6.447 6.672 1.00 0.00 C ATOM 235 C VALA 20144.518 5.816 7.939 1.00 0.00 C ATOM 236 O VALA 20143.685 6.411 8.621 1.00 0.00 O **ATOM** 237 CB VALA 20146.122 7.518 7.065 1.00 0.00 C **ATOM** 238 CG1 VALA 20147.296 6.884 7.795 1.00 0.00 C ATOM 239 CG2 VAL A 20146.598 8.279 5.835 1.00 0.00 C 240 H VALA 20144.013 7.976 5.675 1.00 0.00 H ATOM **ATOM** 241 HA VALA 20145.587 5.685 6.095 1.00 0.00 H **ATOM** 242 HB VALA 20145.648 8.220 7.734 1.00 0.00 H ATOM 243 1HG1 VAL A 20148.120 7.582 7.825 1.00 0.00 H ATOM 244 2HG1 VAL A 20147.602 5.988 7.276 1.00 0.00 H 245 3HG1 VALA 20147.000 6.632 8.802 1.00 0.00 H ATOM 246 1HG2 VAL A 20146.673 9.330 6.069 1.00 0.00 H ATOM 247 2HG2 VAL A 20145.893 8.139 5.029 1.00 0.00 H **ATOM ATOM** 248 3HG2 VALA 20147.567 7.907 5.535 1.00 0.00 H 249 N GLY A 21144.974 4.607 8.247 1.00 0.00 N ATOM 250 CA GLY A 21144.501 3.914 9.431 1.00 0.00 C **ATOM** 251 C GLY A 21143.495 2.828 9.106 1.00 0.00 C ATOM **ATOM** 252 O GLY A 21143.520 1.751 9.699 1.00 0.00 O ATOM 253 H GLY A 21145.639 4.181 7.665 1.00 0.00 H **ATOM** 254 1HA GLY A 21145.347 3.468 9.935 1.00 0.00 H 255 2HA GLY A 21144.040 4.631 10.093 1.00 0.00 H ATOM **ATOM** 256 N SER A 22142.605 3.114 8.159 1.00 0.00 N 257 CA SER A 22141.584 2.153 7.757 1.00 0.00 C ATOM **ATOM** 258 C SER A 22142.168 1.099 6.821 1.00 0.00 C **ATOM** 259 O SER A 22143.084 1.379 6.049 1.00 0.00 O 260 CB SER A 22140.421 2.872 7.070 1.00 0.00 C

261 OG SER A 22139.627 3.571 8.012 1.00 0.00 O 262 H SER A 22142.636 3.990 7.723 1.00 0.00 H **ATOM ATOM** 263 HA SER A 22141.218 1.664 8.647 1.00 0.00 H 264 1HB SER A 22140.810 3.578 6.352 1.00 0.00 H **ATOM** 265 2HB SER A 22139.803 2.146 6.563 1.00 0.00 H **ATOM ATOM** 266 HG SER A 22139.120 4.251 7.562 1.00 0.00 H **ATOM** 267 N LEUA 23141.632 -0.115 6.897 1.00 0.00 N 268 CA LEU A 23142.098 -1.212 6.057 1.00 0.00 C **ATOM** 269 C LEUA 23141.431 -1.171 4.687 1.00 0.00 C **ATOM** 270 O LEUA 23140.263 -0.802 4.564 1.00 0.00 O **ATOM** ATOM 271 CB LEU A 23141.820 -2.555 6.734 1.00 0.00 C **ATOM** 272 CG LEU A 23142.685 -2.855 7.958 1.00 0.00 C 273 CD1 LEU A 23141.930 -3.730 8.945 1.00 0.00 C **ATOM** 274 CD2 LEU A 23143.986 -3.523 7.539 1.00 0.00 C **ATOM** 275 H LEUA 23140.904 -0.277 7.533 1.00 0.00 H **ATOM** 276 HA LEU A 23143.165 -1.098 5.928 1.00 0.00 H **ATOM ATOM** 277 1HB LEU A 23140.783 -2.572 7.039 1.00 0.00 H **ATOM** 278 2HB LEU A 23141.978 -3.339 6.009 1.00 0.00 H 279 HG LEU A 23142.929 -1.927 8.454 1.00 0.00 H **ATOM** 280 1HD1 LEU A 23142.506 -3.832 9.853 1.00 0.00 H **ATOM** 281 2HD1 LEU A 23141.767 -4.705 8.511 1.00 0.00 H **ATOM ATOM** 282 3HD1 LEU A 23140.977 -3.276 9.173 1.00 0.00 H 283 1HD2 LEU A 23144.455 -2.941 6.758 1.00 0.00 H **ATOM** 284 2HD2 LEU A 23143.779 -4.517 7.171 1.00 0.00 H ATOM 285 3HD2 LEU A 23144.650 -3.584 8.389 1.00 0.00 H ATOM 286 N ALAA 24142.180 -1.554 3.658 1.00 0.00 N ATOM ATOM 287 CA ALA A 24141.661 -1.562 2.296 1.00 0.00 C 288 C ALAA 24142.228 -2.732 1.500 1.00 0.00 C ATOM 289 O ALAA 24143.420 -3.033 1.583 1.00 0.00 O ATOM ATOM 290 CB ALA A 24141.979 -0.245 1.603 1.00 0.00 C ATOM 291 H ALAA 24143.104 -1.837 3.819 1.00 0.00 H

- ATOM 292 HA ALA A 24140.587 -1.663 2.349 1.00 0.00 H
- ATOM 293 1HB ALA A 24142.874 -0.358 1.009 1.00 0.00 H
- ATOM 294 2HB ALA A 24142.134 0.524 2.345 1.00 0.00 H
- ATOM 295 3HB ALA A 24141.155 0.033 0.962 1.00 0.00 H
- ATOM 296 N GLU A 25141.369 -3.388 0.727 1.00 0.00 N
- ATOM 297 CA GLU A 25141.786 -4.526 -0.084 1.00 0.00 C
- ATOM 298 C GLU A 25141.885 -4.138 -1.555 1.00 0.00 C
- ATOM 299 O GLU A 25140.962 -3.548 -2.117 1.00 0.00 O
- ATOM 300 CB GLU A 25140.802 -5.686 0.084 1.00 0.00 C
- ATOM 301 CG GLU A 25141.261 -6.974 -0.579 1.00 0.00 C
- ATOM 302 CD GLU A 25140.550 -7.240 -1.891 1.00 0.00 C
- ATOM 303 OE1 GLU A 25140.211 -8.414 -2.155 1.00 0.00 O
- ATOM 304 OE2 GLU A 25140.330 -6.277 -2.654 1.00 0.00 O
- ATOM 305 H GLU A 25140.432 -3.101 0.703 1.00 0.00 H
- ATOM 306 HA GLU A 25142.759 -4.839 0.261 1.00 0.00 H
- ATOM 307 1HB GLU A 25140.665 -5.878 1.138 1.00 0.00 H
- ATOM 308 2HB GLU A 25139.853 -5.403 -0.348 1.00 0.00 H
- ATOM 309 1HG GLU A 25142.322 -6.906 -0.771 1.00 0.00 H
- ATOM 310 2HG GLU A 25141.069 -7.798 0.092 1.00 0.00 H
- ATOM 311 N VAL A 26143.013 -4.472 -2.175 1.00 0.00 N
- ATOM 312 CA VAL A 26143.234 -4.159 -3.582 1.00 0.00 C
- ATOM 313 C VALA 26142.875 -5.344 -4.470 1.00 0.00 C
- ATOM 314 O VALA 26143.102 -6.498 -4.106 1.00 0.00 O
- ATOM 315 CB VAL A 26144.698 -3.759 -3.844 1.00 0.00 C
- ATOM 316 CG1 VAL A 26144.864 -3.239 -5.263 1.00 0.00 C
- ATOM 317 CG2 VAL A 26145.159 -2.722 -2.830 1.00 0.00 C
- ATOM 318 H VALA 26143.712 -4.941 -1.674 1.00 0.00 H
- ATOM 319 HA VAL A 26142.602 -3.322 -3.840 1.00 0.00 H
- ATOM 320 HB VAL A 26145.315 -4.638 -3.733 1.00 0.00 H
- ATOM 321 1HG1 VAL A 26143.919 -2.852 -5.618 1.00 0.00 H
- ATOM 322 2HG1 VAL A 26145.187 -4.044 -5.907 1.00 0.00 H

323 3HG1 VAL A 26145.602 -2.450 -5.274 1.00 0.00 H ATOM ATOM 324 1HG2 VAL A 26145.819 -2.017 -3.312 1.00 0.00 H 325 2HG2 VAL A 26145.683 -3.214 -2.026 1.00 0.00 H ATOM 326 3HG2 VAL A 26144.300 -2.200 -2.434 1.00 0.00 H **ATOM** 327 N LYS A 27142.313 -5.052 -5.639 1.00 0.00 N **ATOM ATOM** 328 CA LYS A 27141.922 -6.094 -6.581 1.00 0.00 C 329 C LYS A 27143.099 -6.503 -7.462 1.00 0.00 C ATOM 330 O LYS A 27143.028 -6.423 -8.689 1.00 0.00 O **ATOM** 331 CB LYS A 27140.758 -5.616 -7.450 1.00 0.00 C ATOM 332 CG LYS A 27139.941 -6.748 -8.051 1.00 0.00 C ATOM **ATOM** 333 CD LYS A 27138.455 -6.426 -8.056 1.00 0.00 C 334 CE LYS A 27138.093 -5.490 -9.199 1.00 0.00 C ATOM 335 NZ LYS A 27136.757 -5.806 -9.773 1.00 0.00 N **ATOM** 336 H LYS A 27142.157 -4.114 -5.874 1.00 0.00 H **ATOM** 337 HA LYS A 27141.603 -6.954 -6.009 1.00 0.00 H **ATOM** ATOM 338 1HB LYS A 27140.100 -5.008 -6.846 1.00 0.00 H 339 2HB LYS A 27141.148 -5.014 -8.257 1.00 0.00 H **ATOM** 340 1HG LYS A 27140.267 -6.913 -9.068 1.00 0.00 H **ATOM** 341 2HG LYS A 27140.104 -7.644 -7.470 1.00 0.00 H **ATOM** 342 1HD LYS A 27137.898 -7.344 -8.166 1.00 0.00 H ATOM 343 2HD LYS A 27138.196 -5.954 -7.120 1.00 0.00 H ATOM **ATOM** 344 1HE LYS A 27138.083 -4.476 -8.826 1.00 0.00 H 345 2HE LYS A 27138.840 -5.581 -9.973 1.00 0.00 H ATOM 346 1HZ LYS A 27136.863 -6.410 -10.613 1.00 0.00 H **ATOM** 347 2HZ LYS A 27136.269 -4.931 -10.049 1.00 0.00 H **ATOM** 348 3HZ LYS A 27136.175 -6.307 -9.072 1.00 0.00 H **ATOM** 349 N GLUA 28144.182 -6.941 -6.829 1.00 0.00 N ATOM 350 CA GLUA 28145.374 -7.363 -7.554 1.00 0.00 C ATOM 351 C GLUA 28145.422 -8.882 -7.682 1.00 0.00 C **ATOM** 352 O GLUA 28144.507 -9.581 -7.248 1.00 0.00 O **ATOM** ATOM 353 CB GLUA 28146.634 -6.857 -6.845 1.00 0.00 C

- ATOM 354 CG GLU A 28147.639 -6.209 -7.782 1.00 0.00 C
- ATOM 355 CD GLUA 28148.605 -5.292 -7.057 1.00 0.00 C
- ATOM 356 OE1 GLU A 28148.525 -4.063 -7.264 1.00 0.00 O
- ATOM 357 OE2 GLU A 28149.440 -5.803 -6.282 1.00 0.00 O
- ATOM 358 H GLUA 28144.179 -6.982 -5.849 1.00 0.00 H
- ATOM 359 HA GLU A 28145.331 -6.931 -8.542 1.00 0.00 H
- ATOM 360 1HB GLU A 28146.346 -6.129 -6.102 1.00 0.00 H
- ATOM 361 2HB GLU A 28147.116 -7.689 -6.354 1.00 0.00 H
- ATOM 362 1HG GLU A 28148.206 -6.984 -8.275 1.00 0.00 H
- ATOM 363 2HG GLU A 28147.103 -5.631 -8.521 1.00 0.00 H
- ATOM 364 N ASN A 29146.495 -9.387 -8.282 1.00 0.00 N
- ATOM 365 CA ASN A 29146.661 -10.823 -8.467 1.00 0.00 C
- ATOM 366 C ASN A 29146.743 -11.539 -7.120 1.00 0.00 C
- ATOM 367 O ASN A 29145.928 -12.410 -6.820 1.00 0.00 O
- ATOM 368 CB ASN A 29147.918 -11.112 -9.291 1.00 0.00 C
- ATOM 369 CG ASN A 29147.608 -11.324 -10.760 1.00 0.00 C
- ATOM 370 OD1 ASN A 29147.598 -12.454 -11.248 1.00 0.00 O
- ATOM 371 ND2 ASN A 29147.356 -10.233 -11.475 1.00 0.00 N
- ATOM 372 H ASN A 29147.192 -8.780 -8.608 1.00 0.00 H
- ATOM 373 HA ASN A 29145.798 -11.190 -9.003 1.00 0.00 H
- ATOM 374 1HB ASN A 29148.598 -10.277 -9.203 1.00 0.00 H
- ATOM 375 2HB ASN A 29148.395 -12.002 -8.910 1.00 0.00 H
- ATOM 376 1HD2 ASN A 29147.382 -9.365 -11.020 1.00 0.00 H
- ATOM 377 2HD2 ASN A 29147.152 -10.341 -12.427 1.00 0.00 H
- ATOM 378 N PRO A 30147.733 -11.175 -6.287 1.00 0.00 N
- ATOM 379 CA PRO A 30147.919 -11.784 -4.967 1.00 0.00 C
- ATOM 380 C PRO A 30146.921 -11.253 -3.938 1.00 0.00 C
- ATOM 381 O PRO A 30147.010 -10.099 -3.519 1.00 0.00 O
- ATOM 382 CB PRO A 30149.341 -11.369 -4.593 1.00 0.00 C
- ATOM 383 CG PRO A 30149.544 -10.067 -5.286 1.00 0.00 C
- ATOM 384 CD PRO A 30148.751 -10.141 -6.565 1.00 0.00 C

385 HA PRO A 30147.855 -12.860 -5.014 1.00 0.00 H **ATOM** 386 1HB PRO A 30149.419 -11.265 -3.521 1.00 0.00 H **ATOM** 387 2HB PRO A 30150.040 -12.115 -4.942 1.00 0.00 H ATOM 388 1HG PRO A 30149.181 -9.261 -4.667 1.00 0.00 H **ATOM** 389 2HG PRO A 30150.593 -9.927 -5.506 1.00 0.00 H **ATOM** 390 1HD PRO A 30148.285 -9.191 -6.775 1.00 0.00 H **ATOM** 391 2HD PRO A 30149.386 -10.439 -7.385 1.00 0.00 H ATOM 392 N PRO A 31145.956 -12.087 -3.514 1.00 0.00 N ATOM 393 CA PRO A 31144.946 -11.687 -2.529 1.00 0.00 C **ATOM** 394 C PRO A 31145.541 -11.490 -1.138 1.00 0.00 C **ATOM** 395 O PRO A 31145.621 -12.431 -0.349 1.00 0.00 O **ATOM** 396 CB PRO A 31143.962 -12.857 -2.529 1.00 0.00 C **ATOM** 397 CG PRO A 31144.764 -14.027 -2.981 1.00 0.00 C **ATOM** 398 CD PRO A 31145.771 -13.483 -3.957 1.00 0.00 C **ATOM** 399 HA PRO A 31144.436 -10.783 -2.831 1.00 0.00 H **ATOM** ATOM 400 1HB PRO A 31143.574 -13.006 -1.531 1.00 0.00 H 401 2HB PRO A 31143.149 -12.649 -3.209 1.00 0.00 H ATOM 402 1HG PRO A 31145.264 -14.479 -2.137 1.00 0.00 H **ATOM** 403 2HG PRO A 31144.123 -14.746 -3.468 1.00 0.00 H ATOM 404 1HD PRO A 31146.697 -14.035 -3.889 1.00 0.00 H **ATOM** 405 2HD PRO A 31145.380 -13.519 -4.963 1.00 0.00 H **ATOM ATOM** 406 N PHE A 32145.954 -10.262 -0.844 1.00 0.00 N 407 CA PHE A 32146.541 -9.942 0.452 1.00 0.00 C **ATOM** 408 C PHE A 32145.685 -8.925 1.201 1.00 0.00 C **ATOM** 409 O PHE A 32144.726 -8.383 0.652 1.00 0.00 O ATOM 410 CB PHE A 32147.959 -9.398 0.273 1.00 0.00 C **ATOM** 411 CG PHE A 32148.045 -8.250 -0.693 1.00 0.00 C ATOM 412 CD1 PHE A 32148.676 -8.404 -1.917 1.00 0.00 C ATOM 413 CD2 PHE A 32147.495 -7.019 -0.376 1.00 0.00 C ATOM 414 CE1 PHE A 32148.757 -7.350 -2.808 1.00 0.00 C **ATOM** ATOM 415 CE2 PHE A 32147.573 -5.962 -1.262 1.00 0.00 C

416 CZ PHEA 32148.205 -6.127 -2.480 1.00 0.00 C 417 H PHE A 32145.862 -9.553 -1.515 1.00 0.00 H **ATOM** 418 HA PHE A 32146.585 -10.853 1.030 1.00 0.00 H **ATOM** 419 1HB PHE A 32148.329 -9.056 1.228 1.00 0.00 H **ATOM** 420 2HB PHE A 32148.597 -10.190 -0.093 1.00 0.00 H **ATOM** 421 HD1 PHE A 32149.108 -9.360 -2.174 1.00 0.00 H **ATOM ATOM** 422 HD2 PHE A 32147.001 -6.889 0.575 1.00 0.00 H **ATOM** 423 HE1 PHE A 32149.252 -7.482 -3.758 1.00 0.00 H 424 HE2 PHE A 32147.140 -5.006 -1.004 1.00 0.00 H **ATOM** 425 HZ PHE A 32148.266 -5.302 -3.174 1.00 0.00 H **ATOM** 426 N TYR A 33146.038 -8.673 2.456 1.00 0.00 N **ATOM ATOM** 427 CA TYR A 33145.302 -7.722 3.281 1.00 0.00 C 428 C TYR A 33146.253 -6.758 3.983 1.00 0.00 C ATOM 429 O TYR A 33147.107 -7.174 4.765 1.00 0.00 O ATOM 430 CB TYR A 33144.453 -8.462 4.315 1.00 0.00 C **ATOM** ATOM 431 CG TYR A 33143.141 -8.978 3.767 1.00 0.00 C **ATOM** 432 CD1 TYR A 33142.756 -10.298 3.963 1.00 0.00 C 433 CD2 TYR A 33142.290 -8.145 3.051 1.00 0.00 C ATOM 434 CE1 TYR A 33141.559 -10.773 3.462 1.00 0.00 C ATOM **ATOM** 435 CE2 TYR A 33141.092 -8.612 2.547 1.00 0.00 C 436 CZ TYR A 33140.731 -9.927 2.755 1.00 0.00 C **ATOM ATOM** 437 OH TYR A 33139.538 -10.397 2.256 1.00 0.00 O 438 H TYR A 33146.812 -9.137 2.838 1.00 0.00 H **ATOM** 439 HA TYR A 33144.650 -7.156 2.632 1.00 0.00 H ATOM 440 1HB TYR A 33145.010 -9.308 4.690 1.00 0.00 H ATOM 441 2HB TYR A 33144.231 -7.793 5.134 1.00 0.00 H ATOM 442 HD1 TYR A 33143,406 -10.958 4.516 1.00 0.00 H ATOM ATOM 443 HD2 TYR A 33142.577 -7.116 2.889 1.00 0.00 H 444 HE1 TYR A 33141.276 -11.802 3.625 1.00 0.00 H ATOM 445 HE2 TYR A 33140.443 -7.949 1.995 1.00 0.00 H ATOM ATOM 446 HH TYR A 33139.663 -11.281 1.906 1.00 0.00 H

- ATOM 447 N GLY A 34146.099 -5.469 3.698 1.00 0.00 N
- ATOM 448 CA GLY A 34146.951 -4.466 4.310 1.00 0.00 C
- ATOM 449 C GLY A 34146.174 -3.251 4.775 1.00 0.00 C
- ATOM 450 O GLY A 34144.997 -3.095 4.450 1.00 0.00 O
- ATOM 451 H GLY A 34145.401 -5.196 3.066 1.00 0.00 H
- ATOM 452 1HA GLY A 34147.453 -4.907 5.160 1.00 0.00 H
- ATOM 453 2HA GLY A 34147.693 -4.153 3.591 1.00 0.00 H
- ATOM 454 N VALA 35146.834 -2.386 5.539 1.00 0.00 N
- ATOM 455 CA VALA 35146.199 -1.178 6.051 1.00 0.00 C
- ATOM 456 C VALA 35146.808 0.071 5.421 1.00 0.00 C
- ATOM 457 O VALA 35148.011 0.125 5.164 1.00 0.00 O
- ATOM 458 CB VALA 35146.323 -1.085 7.585 1.00 0.00 C
- ATOM 459 CG1 VAL A 35147.784 -1.017 8.004 1.00 0.00 C
- ATOM 460 CG2 VAL A 35145.552 0.115 8.113 1.00 0.00 C
- ATOM 461 H VALA 35147.771 -2.566 5.764 1.00 0.00 H
- ATOM 462 HA VAL A 35145.150 -1.221 5.797 1.00 0.00 H
- ATOM 463 HB VAL A 35145.892 -1.978 8.014 1.00 0.00 H
- ATOM 464 1HG1 VAL A 35148.204 -0.071 7.695 1.00 0.00 H
- ATOM 465 2HG1 VAL A 35148.330 -1.823 7.536 1.00 0.00 H
- ATOM 466 3HG1 VAL A 35147.856 -1.109 9.077 1.00 0.00 H
- ATOM 467 1HG2 VAL A 35145.807 0.279 9.150 1.00 0.00 H
- ATOM 468 2HG2 VAL A 35144.492 -0.072 8.028 1.00 0.00 H
- ATOM 469 3HG2 VAL A 35145.810 0.992 7.536 1.00 0.00 H
- ATOM 470 N ILE A 36145.971 1.073 5.176 1.00 0.00 N
- ATOM 471 CA ILE A 36146.429 2.321 4.577 1.00 0.00 C
- ATOM 472 C ILE A 36147.374 3.064 5.516 1.00 0.00 C
- ATOM 473 O ILE A 36147.092 3.216 6.705 1.00 0.00 O
- ATOM 474 CB ILE A 36145.246 3.243 4.222 1.00 0.00 C
- ATOM 475 CG1 ILE A 36144.208 2.484 3.392 1.00 0.00 C
- ATOM 476 CG2 ILE A 36145.738 4.471 3.468 1.00 0.00 C
- ATOM 477 CD1 ILE A 36142.999 3.317 3.025 1.00 0.00 C

478 H ILE A 36145.024 0.971 5.403 1.00 0.00 H **ATOM** 479 HA ILE A 36146.957 2.080 3.666 1.00 0.00 H **ATOM** 480 HB ILE A 36144.788 3.577 5.141 1.00 0.00 H **ATOM ATOM** 481 1HG1 ILE A 36144.667 2.145 2.476 1.00 0.00 H 482 2HG1 ILE A 36143.863 1.628 3.955 1.00 0.00 H **ATOM** 483 1HG2 ILE A 36145.851 5.295 4.157 1.00 0.00 H ATOM 484 2HG2 ILE A 36145.022 4.736 2.703 1.00 0.00 H **ATOM ATOM** 485 3HG2 ILE A 36146.690 4.253 3.008 1.00 0.00 H 486 1HD1 ILE A 36143.202 4.357 3.236 1.00 0.00 H **ATOM** 487 2HD1 ILE A 36142.148 2.992 3.605 1.00 0.00 H ATOM **ATOM** 488 3HD1 ILE A 36142.786 3.198 1.974 1.00 0.00 H 489 N ARG A 37148.499 3.521 4.974 1.00 0.00 N **ATOM** 490 CA ARG A 37149.487 4.246 5.763 1.00 0.00 C ATOM 491 C ARG A 37149.637 5.680 5.265 1.00 0.00 C **ATOM** 492 O ARG A 37149.354 6.632 5.992 1.00 0.00 O ATOM 493 CB ARG A 37150.838 3.530 5.706 1.00 0.00 C ATOM 494 CG ARG A 37150.753 2.046 6.021 1.00 0.00 C **ATOM** 495 CD ARG A 37150.195 1.803 7.414 1.00 0.00 C ATOM **ATOM** 496 NE ARG A 37151.099 2.281 8.457 1.00 0.00 N 497 CZ ARG A 37150.986 1.952 9.743 1.00 0.00 C **ATOM** 498 NH1 ARG A 37150.012 1.148 10.146 1.00 0.00 N **ATOM** 499 NH2 ARG A 37151.853 2.429 10.626 1.00 0.00 N **ATOM** 500 H ARG A 37148.667 3.368 4.021 1.00 0.00 H **ATOM** 501 HA ARG A 37149.145 4.267 6.787 1.00 0.00 H **ATOM** 502 1HB ARG A 37151.251 3.643 4.714 1.00 0.00 H **ATOM** 503 2HB ARG A 37151.507 3.990 6.419 1.00 0.00 H ATOM 504 1HG ARG A 37150.108 1.570 5.298 1.00 0.00 H **ATOM** 505 2HG ARG A 37151.743 1.618 5.960 1.00 0.00 H ATOM 506 1HD ARG A 37149.251 2.321 7.505 1.00 0.00 H **ATOM ATOM** 507 2HD ARG A 37150.037 0.742 7.545 1.00 0.00 H 508 HE ARGA 37151.828 2.877 8.187 1.00 0.00 H ATOM

ATOM 509 1HH1 ARG A 37149.355 0.785 9.486 1.00 0.00 H **ATOM** 510 2HH1 ARG A 37149.933 0.905 11.114 1.00 0.00 H 511 1HH2 ARG A 37152.590 3.035 10.327 1.00 0.00 H **ATOM** 512 2HH2 ARG A 37151.769 2.182 11.592 1.00 0.00 H ATOM **ATOM** 513 N TRPA 38150.084 5.827 4.022 1.00 0.00 N ATOM 514 CA TRP A 38150.270 7.146 3.428 1.00 0.00 C 515 C TRPA 38149.501 7.268 2.117 1.00 0.00 C **ATOM ATOM** 516 O TRP A 38149.565 6.385 1.262 1.00 0.00 O 517 CB TRP A 38151.761 7.418 3.190 1.00 0.00 C **ATOM** ATOM 518 CG TRP A 38152.021 8.634 2.350 1.00 0.00 C **ATOM** 519 CD1 TRP A 38152.212 9.911 2.791 1.00 0.00 C 520 CD2 TRP A 38152.116 8.683 0.922 1.00 0.00 C **ATOM** 521 NE1 TRP A 38152.417 10.753 1.725 1.00 0.00 N **ATOM** 522 CE2 TRP A 38152.363 10.022 0.565 1.00 0.00 C **ATOM** 523 CE3 TRP A 38152.014 7.725 -0.090 1.00 0.00 C ATOM **ATOM** 524 CZ2 TRP A 38152.511 10.424 -0.760 1.00 0.00 C 525 CZ3 TRP A 38152.162 8.125 -1.405 1.00 0.00 C ATOM 526 CH2 TRP A 38152.408 9.465 -1.729 1.00 0.00 C **ATOM** 527 H TRP A 38150.293 5.030 3.491 1.00 0.00 H ATOM 528 HA TRP A 38149.888 7.879 4.123 1.00 0.00 H ATOM ATOM 529 1HB TRP A 38152.250 7.560 4.142 1.00 0.00 H **ATOM** 530 2HB TRP A 38152.198 6.566 2.690 1.00 0.00 H 531 HD1 TRP A 38152.198 10.204 3.831 1.00 0.00 H ATOM 532 HE1 TRP A 38152.577 11.718 1.783 1.00 0.00 H **ATOM** 533 HE3 TRP A 38151.825 6.687 0.140 1.00 0.00 H ATOM 534 HZ2 TRP A 38152.699 11.454 -1.027 1.00 0.00 H **ATOM** 535 HZ3 TRP A 38152.087 7.398 -2.200 1.00 0.00 H ATOM 536 HH2 TRP A 38152.516 9.733 -2.771 1.00 0.00 H ATOM 537 N ILE A 39148.781 8.374 1.963 1.00 0.00 N ATOM 538 CA ILE A 39148.004 8.624 0.756 1.00 0.00 C ATOM ATOM 539 C ILE A 39148.406 9.950 0.121 1.00 0.00 C

ATOM 540 O ILE A 39148.069 11.019 0.631 1.00 0.00 O 541 CB ILE A 39146.492 8.645 1.051 1.00 0.00 C 542 CG1 ILE A 39146.088 7.406 1.853 1.00 0.00 C **ATOM** 543 CG2 ILE A 39145.699 8.725 -0.245 1.00 0.00 C ATOM **ATOM** 544 CD1 ILE A 39144.772 7.560 2.583 1.00 0.00 C 545 H ILE A 39148.776 9.043 2.680 1.00 0.00 H ATOM 546 HA ILE A 39148.205 7.824 0.056 1.00 0.00 H **ATOM** ATOM 547 HB ILE A 39146.274 9.527 1.633 1.00 0.00 H 548 1HG1 ILE A 39145.997 6.564 1.182 1.00 0.00 H ATOM **ATOM** 549 2HG1 ILE A 39146.852 7.195 2.587 1.00 0.00 H 550 1HG2 ILE A 39144.687 9.034 -0.029 1.00 0.00 H ATOM 551 2HG2 ILE A 39145.686 7.756 -0.720 1.00 0.00 H ATOM ATOM 552 3HG2 ILE A 39146.162 9.443 -0.905 1.00 0.00 H 553 1HD1 ILE A 39144.751 8.514 3.089 1.00 0.00 H ATOM 554 2HD1 ILE A 39144.666 6.766 3.306 1.00 0.00 H ATOM 555 3HD1 ILE A 39143.960 7.512 1.874 1.00 0.00 H ATOM 556 N GLY A 40149.135 9.876 -0.987 1.00 0.00 N ATOM 557 CA GLY A 40149.575 11.083 -1.663 1.00 0.00 C **ATOM** 558 C GLY A 40150.097 10.816 -3.060 1.00 0.00 C ATOM 559 O GLY A 40149.921 9.724 -3.600 1.00 0.00 O ATOM 560 H GLY A 40149.378 8.997 -1.348 1.00 0.00 H ATOM 561 1HA GLY A 40148.745 11.769 -1.727 1.00 0.00 H ATOM ATOM 562 2HA GLY A 40150.359 11.540 -1.079 1.00 0.00 H 563 N GLN A 41150.741 11.820 -3.644 1.00 0.00 N ATOM 564 CA GLN A 41151.294 11.701 -4.987 1.00 0.00 C ATOM 565 C GLN A 41152.768 12.102 -5.001 1.00 0.00 C ATOM 566 O GLN A 41153.105 13.259 -4.749 1.00 0.00 O ATOM 567 CB GLN A 41150.504 12.581 -5.956 1.00 0.00 C ATOM 568 CG GLN A 41148.998 12.402 -5.849 1.00 0.00 C **ATOM** 569 CD GLN A 41148.246 13.712 -5.972 1.00 0.00 C ATOM ATOM 570 OE1 GLN A 41148.223 14.518 -5.040 1.00 0.00 O **ATOM** 571 NE2 GLN A 41147.627 13.933 -7.125 1.00 0.00 N 572 H GLN A 41150.847 12.665 -3.160 1.00 0.00 H **ATOM ATOM** 573 HA GLN A 41151.205 10.672 -5.295 1.00 0.00 H 574 1HB GLN A 41150.737 13.616 -5.753 1.00 0.00 H **ATOM ATOM** 575 2HB GLN A 41150.804 12.344 -6.964 1.00 0.00 H 576 1HG GLN A 41148.670 11.741 -6.637 1.00 0.00 H ATOM 577 2HG GLN A 41148.767 11.960 -4.891 1.00 0.00 H ATOM 578 1HE2 GLN A 41147.689 13.246 -7.822 1.00 0.00 H ATOM 579 2HE2 GLN A 41147.135 14.773 -7.233 1.00 0.00 H **ATOM** ATOM 580 N PRO A 42153.674 11.150 -5.295 1.00 0.00 N 581 CA PRO A 42155.115 11.422 -5.336 1.00 0.00 C **ATOM** 582 C PRO A 42155.468 12.529 -6.324 1.00 0.00 C **ATOM** 583 O PRO A 42154.696 12.830 -7.233 1.00 0.00 O **ATOM** 584 CB PRO A 42155.723 10.089 -5.787 1.00 0.00 C **ATOM ATOM** 585 CG PRO A 42154.699 9.066 -5.440 1.00 0.00 C **ATOM** 586 CD PRO A 42153.371 9.743 -5.609 1.00 0.00 C 587 HA PRO A 42155.495 11.680 -4.358 1.00 0.00 H ATOM 588 1HB PRO A 42155.909 10.118 -6.851 1.00 0.00 H **ATOM** 589 2HB PRO A 42156.648 9.915 -5.259 1.00 0.00 H ATOM 590 1HG PRO A 42154.778 8.222 -6.110 1.00 0.00 H ATOM 591 2HG PRO A 42154.830 8.746 -4.416 1.00 0.00 H ATOM 592 1HD PRO A 42153.021 9.641 -6.626 1.00 0.00 H ATOM 593 2HD PRO A 42152.648 9.341 -4.916 1.00 0.00 H **ATOM** 594 N PRO A 43156.647 13.151 -6.158 1.00 0.00 N ATOM 595 CA PRO A 43157.102 14.228 -7.040 1.00 0.00 C ATOM 596 C PRO A 43157.497 13.719 -8.421 1.00 0.00 C **ATOM** 597 O PRO A 43158.662 13.408 -8.668 1.00 0.00 O ATOM 598 CB PRO A 43158.322 14.792 -6.312 1.00 0.00 C ATOM 599 CG PRO A 43158.835 13.657 -5.497 1.00 0.00 C **ATOM** 600 CD PRO A 43157.629 12.850 -5.098 1.00 0.00 C **ATOM** 601 HA PRO A 43156.351 14.999 -7.142 1.00 0.00 H ATOM

602 1HB PRO A 43159.052 15.121 -7.037 1.00 0.00 H ATOM 603 2HB PRO A 43158.023 15.622 -5.691 1.00 0.00 H ATOM ATOM 604 1HG PRO A 43159.510 13.056 -6.088 1.00 0.00 H **ATOM** 605 2HG PRO A 43159.339 14.035 -4.619 1.00 0.00 H 606 1HD PRO A 43157.869 11.797 -5.082 1.00 0.00 H ATOM 607 2HD PRO A 43157.264 13.170 -4.134 1.00 0.00 H ATOM ATOM 608 N GLY A 44156.521 13.636 -9.317 1.00 0.00 N 609 CA GLY A 44156.790 13.162 -10.661 1.00 0.00 C ATOM 610 C GLY A 44155.552 12.623 -11.346 1.00 0.00 C ATOM 611 O GLYA 44155.237 13.014 -12.471 1.00 0.00 O **ATOM** 612 H GLY A 44155.610 13.897 -9.064 1.00 0.00 H **ATOM** 613 1HA GLY A 44157.183 13.980 -11.245 1.00 0.00 H ATOM 614 2HA GLY A 44157.532 12.380 -10.613 1.00 0.00 H ATOM ATOM 615 N LEU A 45154.848 11.724 -10.670 1.00 0.00 N 616 CA LEU A 45153.637 11.131 -11.224 1.00 0.00 C ATOM 617 C LEUA 45152.440 11.401 -10.319 1.00 0.00 C ATOM ATOM 618 O LEUA 45152.369 10.888 -9.203 1.00 0.00 O 619 CB LEU A 45153.820 9.623 -11.409 1.00 0.00 C **ATOM** ATOM 620 CG LEU A 45154.384 8.886 -10.192 1.00 0.00 C ATOM 621 CD1 LEU A 45154.025 7.407 -10.247 1.00 0.00 C 622 CD2 LEU A 45155.893 9.072 -10.107 1.00 0.00 C ATOM 623 H LEUA 45155.148 11.452 -9.775 1.00 0.00 H ATOM 624 HA LEU A 45153.455 11.583 -12.186 1.00 0.00 H ATOM 625 1HB LEU A 45152.860 9.192 -11.653 1.00 0.00 H **ATOM** 626 2HB LEU A 45154.490 9.462 -12.240 1.00 0.00 H ATOM 627 HG LEU A 45153.945 9.301 -9.295 1.00 0.00 H ATOM 628 1HD1 LEU A 45153.490 7.134 -9.349 1.00 0.00 H ATOM ATOM 629 2HD1 LEU A 45154.928 6.819 -10.320 1.00 0.00 H 630 3HD1 LEU A 45153.402 7.218 -11.108 1.00 0.00 H ATOM 631 1HD2 LEU A 45156.162 9.381 -9.108 1.00 0.00 H ATOM 632 2HD2 LEU A 45156.205 9.827 -10.813 1.00 0.00 H ATOM

ATOM 633 3HD2 LEU A 45156.385 8.138 -10.339 1.00 0.00 H 634 N ASN A 46151.505 12.210 -10.803 1.00 0.00 N **ATOM** 635 CA ASN A 46150.318 12.539 -10.025 1.00 0.00 C **ATOM** 636 C ASN A 46149.367 11.349 -9.971 1.00 0.00 C **ATOM** 637 O ASN A 46148.723 11.008 -10.964 1.00 0.00 O ATOM 638 CB ASN A 46149.608 13.751 -10.630 1.00 0.00 C **ATOM ATOM** 639 CG ASN A 46148.879 14.574 -9.586 1.00 0.00 C **ATOM** 640 OD1 ASN A 46147.654 14.691 -9.615 1.00 0.00 O 641 ND2 ASN A 46149.632 15.152 -8.657 1.00 0.00 N **ATOM** 642 H ASN A 46151.613 12.592 -11.699 1.00 0.00 H **ATOM** ATOM 643 HA ASN A 46150.633 12.780 -9.020 1.00 0.00 H **ATOM** 644 1HB ASN A 46150.337 14.383 -11.114 1.00 0.00 H 645 2HB ASN A 46148.889 13.411 -11.361 1.00 0.00 H **ATOM** 646 1HD2 ASN A 46150.602 15.015 -8.696 1.00 0.00 H **ATOM** 647 2HD2 ASN A 46149.188 15.690 -7.970 1.00 0.00 H **ATOM** ATOM 648 N GLUA 47149.285 10.721 -8.804 1.00 0.00 N **ATOM** 649 CA GLU A 47148.415 9.568 -8.612 1.00 0.00 C 650 C GLUA 47148.262 9.248 -7.130 1.00 0.00 C **ATOM** 651 O GLUA 47149.245 8.978 -6.440 1.00 0.00 O **ATOM ATOM** 652 CB GLU A 47148.970 8.349 -9.354 1.00 0.00 C 653 CG GLU A 47150.485 8.230 -9.290 1.00 0.00 C **ATOM ATOM** 654 CD GLU A 47151.036 7.254 -10.311 1.00 0.00 C 655 OE1 GLU A 47151.168 7.641 -11.491 1.00 0.00 O **ATOM** 656 OE2 GLU A 47151.336 6.103 -9.930 1.00 0.00 O **ATOM ATOM** 657 H GLU A 47149.824 11.041 -8.052 1.00 0.00 H ATOM 658 HA GLU A 47147.445 9.813 -9.017 1.00 0.00 H 659 1HB GLU A 47148.543 7.455 -8.923 1.00 0.00 H ATOM **ATOM** 660 2HB GLU A 47148.680 8.411 -10.392 1.00 0.00 H

661 1HG GLUA 47150.917 9.201 -9.474 1.00 0.00 H

662 2HG GLUA 47150.767 7.894 -8.303 1.00 0.00 H

ATOM 663 N VALA 48147.026 9.273 -6.644 1.00 0.00 N

ATOM

ATOM

- ATOM 664 CA VALA 48146.758 8.977 -5.243 1.00 0.00 C
- ATOM 665 C VALA 48147.120 7.533 -4.918 1.00 0.00 C
- ATOM 666 O VALA 48146.338 6.615 -5.169 1.00 0.00 O
- ATOM 667 CB VALA 48145.279 9.219 -4.888 1.00 0.00 C
- ATOM 668 CG1 VAL A 48145.066 9.114 -3.386 1.00 0.00 C
- ATOM 669 CG2 VAL A 48144.820 10.574 -5.405 1.00 0.00 C
- ATOM 670 H VALA 48146.280 9.489 -7.241 1.00 0.00 H
- ATOM 671 HA VALA 48147.366 9.636 -4.640 1.00 0.00 H
- ATOM 672 HB VAL A 48144.684 8.455 -5.368 1.00 0.00 H
- ATOM 673 1HG1 VAL A 48145.014 8.072 -3.102 1.00 0.00 H
- ATOM 674 2HG1 VALA 48144.142 9.606 -3.117 1.00 0.00 H
- ATOM 675 3HG1 VAL A 48145.889 9.587 -2.872 1.00 0.00 H
- ATOM 676 1HG2 VAL A 48144.651 10.515 -6.470 1.00 0.00 H
- ATOM 677 2HG2 VAL A 48145.580 11.314 -5.202 1.00 0.00 H
- ATOM 678 3HG2 VAL A 48143.903 10.857 -4.910 1.00 0.00 H
- ATOM 679 N LEUA 49148.309 7.339 -4.362 1.00 0.00 N
- ATOM 680 CA LEU A 49148.777 6.005 -4.005 1.00 0.00 C
- ATOM 681 C LEU A 49148.742 5.809 -2.496 1.00 0.00 C
- ATOM 682 O LEUA 49149.455 6.486 -1.756 1.00 0.00 O
- ATOM 683 CB LEU A 49150.197 5.781 -4.528 1.00 0.00 C
- ATOM 684 CG LEU A 49150.343 5.837 -6.050 1.00 0.00 C
- ATOM 685 CD1 LEU A 49151.745 6.281 -6.435 1.00 0.00 C
- ATOM 686 CD2 LEU A 49150.022 4.483 -6.664 1.00 0.00 C
- ATOM 687 H LEUA 49148.888 8.110 -4.186 1.00 0.00 H
- ATOM 688 HA LEU A 49148.115 5.287 -4.466 1.00 0.00 H
- ATOM 689 1HB LEU A 49150.840 6.535 -4.097 1.00 0.00 H
- ATOM 690 2HB LEU A 49150.532 4.812 -4.192 1.00 0.00 H
- ATOM 691 HG LEU A 49149.643 6.559 -6.446 1.00 0.00 H
- ATOM 692 1HD1 LEU A 49151.964 7.230 -5.968 1.00 0.00 H
- ATOM 693 2HD1 LEU A 49151.808 6.384 -7.507 1.00 0.00 H
- ATOM 694 3HD1 LEU A 49152.461 5.543 -6.102 1.00 0.00 H

- ATOM 695 1HD2 LEU A 49149.950 4.582 -7.737 1.00 0.00 H
- ATOM 696 2HD2 LEU A 49149.083 4.122 -6.272 1.00 0.00 H
- ATOM 697 3HD2 LEU A 49150.807 3.782 -6.420 1.00 0.00 H
- ATOM 698 N ALA A 50147.908 4.880 -2.044 1.00 0.00 N
- ATOM 699 CA ALA A 50147.783 4.602 -0.621 1.00 0.00 C
- ATOM 700 C ALA A 50148.733 3.488 -0.195 1.00 0.00 C
- ATOM 701 O ALA A 50148.596 2.343 -0.625 1.00 0.00 O
- ATOM 702 CB ALA A 50146.347 4.234 -0.280 1.00 0.00 C
- ATOM 703 H ALA A 50147.363 4.374 -2.682 1.00 0.00 H
- ATOM 704 HA ALA A 50148.036 5.505 -0.086 1.00 0.00 H
- ATOM 705 1HB ALA A 50146.227 3.162 -0.329 1.00 0.00 H
- ATOM 706 2HB ALA A 50145.677 4.704 -0.985 1.00 0.00 H
- ATOM 707 3HB ALA A 50146.115 4.577 0.718 1.00 0.00 H
- ATOM 708 N GLY A 51149.697 3.832 0.653 1.00 0.00 N
- ATOM 709 CA GLY A 51150.656 2.850 1.123 1.00 0.00 C
- ATOM 710 C GLY A 51150.023 1.805 2.019 1.00 0.00 C
- ATOM 711 O GLY A 51149.665 2.092 3.162 1.00 0.00 O
- ATOM 712 H GLY A 51149.757 4.759 0.962 1.00 0.00 H
- ATOM 713 1HA GLY A 51151.098 2.357 0.270 1.00 0.00 H
- ATOM 714 2HA GLY A 51151.434 3.357 1.674 1.00 0.00 H
- ATOM 715 N LEU A 52149.882 0.589 1.501 1.00 0.00 N
- ATOM 716 CA LEU A 52149.286 -0.502 2.264 1.00 0.00 C
- ATOM 717 C LEUA 52150.362 -1.350 2.933 1.00 0.00 C
- ATOM 718 O LEUA 52151.348 -1.734 2.303 1.00 0.00 O
- ATOM 719 CB LEU A 52148.423 -1.376 1.353 1.00 0.00 C
- ATOM 720 CG LEU A 52147.132 -0.721 0.860 1.00 0.00 C
- ATOM 721 CD1 LEU A 52146.434 -1.615 -0.154 1.00 0.00 C
- ATOM 722 CD2 LEU A 52146.209 -0.418 2.031 1.00 0.00 C
- ATOM 723 H LEUA 52150.186 0.422 0.585 1.00 0.00 H
- ATOM 724 HA LEU A 52148.660 -0.067 3.029 1.00 0.00 H
- ATOM 725 1HB LEU A 52149.014 -1.654 0.492 1.00 0.00 H

726 2HB LEU A 52148.162 -2.274 1.893 1.00 0.00 H ATOM **ATOM** 727 HG LEU A 52147.372 0.212 0.373 1.00 0.00 H 728 1HD1 LEU A 52147.160 -2.260 -0.625 1.00 0.00 H ATOM 729 2HD1 LEU A 52145.957 -1.002 -0.905 1.00 0.00 H **ATOM** 730 3HD1 LEU A 52145.689 -2.215 0.348 1.00 0.00 H ATOM 731 1HD2 LEU A 52146.708 0.245 2.721 1.00 0.00 H **ATOM** ATOM 732 2HD2 LEU A 52145.955 -1.339 2.536 1.00 0.00 H 733 3HD2 LEU A 52145.308 0.053 1.666 1.00 0.00 H ATOM **ATOM** 734 N GLUA 53150.166 -1.641 4.216 1.00 0.00 N 735 CA GLU A 53151.119 -2.445 4.972 1.00 0.00 C ATOM 736 C GLUA 53150.624 -3.880 5.117 1.00 0.00 C ATOM 737 O GLUA 53149.715 -4.158 5.899 1.00 0.00 O **ATOM** ATOM 738 CB GLU A 53151.353 -1.830 6.353 1.00 0.00 C 739 CG GLUA 53152.363 -2.593 7.195 1.00 0.00 C **ATOM** 740 CD GLUA 53151.997 -2.614 8.666 1.00 0.00 C **ATOM** 741 OE1 GLU A 53152.380 -3.580 9.360 1.00 0.00 O ATOM 742 OE2 GLU A 53151.327 -1.665 9.126 1.00 0.00 O **ATOM** ATOM 743 H GLU A 53149.362 -1.306 4.663 1.00 0.00 H 744 HA GLUA 53152.053 -2.451 4.428 1.00 0.00 H **ATOM** 745 1HB GLU A 53151.710 -0.819 6.229 1.00 0.00 H **ATOM** 746 2HB GLU A 53150.414 -1.808 6.887 1.00 0.00 H **ATOM** 747 1HG GLU A 53152.415 -3.610 6.838 1.00 0.00 H ATOM 748 2HG GLU A 53153.330 -2.124 7.086 1.00 0.00 H **ATOM ATOM** 749 N LEUA 54151.229 -4.789 4.359 1.00 0.00 N 750 CA LEU A 54150.850 -6.196 4.403 1.00 0.00 C ATOM 751 C LEUA 54151.179 -6.805 5.763 1.00 0.00 C **ATOM** 752 O LEUA 54152.268 -6.599 6.300 1.00 0.00 O **ATOM** 753 CB LEU A 54151.564 -6.973 3.296 1.00 0.00 C **ATOM** 754 CG LEUA 54151.397 -6.396 1.889 1.00 0.00 C **ATOM** 755 CD1 LEU A 54152.493 -6.907 0.968 1.00 0.00 C **ATOM** 756 CD2 LEU A 54150.025 -6.742 1.331 1.00 0.00 C ATOM

757 H LEUA 54151.948 -4.506 3.755 1.00 0.00 H ATOM **ATOM** 758 HA LEU A 54149.784 -6.257 4.244 1.00 0.00 H ATOM 759 1HB LEU A 54152.618 -7.003 3.529 1.00 0.00 H 760 2HB LEU A 54151.183 -7.984 3.293 1.00 0.00 H **ATOM** ATOM 761 HG LEU A 54151.478 -5.319 1.938 1.00 0.00 H 762 1HD1 LEU A 54153.458 -6.635 1.372 1.00 0.00 H ATOM ATOM 763 2HD1 LEU A 54152.376 -6.467 -0.011 1.00 0.00 H 764 3HD1 LEU A 54152.426 -7.982 0.891 1.00 0.00 H ATOM **ATOM** 765 1HD2 LEU A 54149.885 -7.812 1.357 1.00 0.00 H 766 2HD2 LEU A 54149.953 -6.394 0.312 1.00 0.00 H **ATOM** 767 3HD2 LEU A 54149.262 -6.266 1.929 1.00 0.00 H **ATOM ATOM** 768 N GLUA 55150.231 -7.556 6.314 1.00 0.00 N 769 CA GLU A 55150.420 -8.196 7.610 1.00 0.00 C **ATOM** 770 C GLUA 55151.540 -9.230 7.551 1.00 0.00 C **ATOM** 771 O GLUA 55152.232 -9.466 8.542 1.00 0.00 O **ATOM** 772 CB GLU A 55149.120 -8.861 8.068 1.00 0.00 C ATOM 773 CG GLU A 55148.144 -7.900 8.725 1.00 0.00 C **ATOM** 774 CD GLUA 55148.143 -8.013 10.237 1.00 0.00 C ATOM 775 OE1 GLU A 55149.238 -7.979 10.837 1.00 0.00 O ATOM ATOM 776 OE2 GLU A 55147.046 -8.137 10.823 1.00 0.00 O 777 H GLUA 55149.385 -7.684 5.837 1.00 0.00 H ATOM 778 HA GLU A 55150.690 -7.429 8.321 1.00 0.00 H ATOM ATOM 779 1HB GLU A 55148.635 -9.303 7.210 1.00 0.00 H 780 2HB GLU A 55149.358 -9.639 8.778 1.00 0.00 H **ATOM** 781 1HG GLU A 55148.415 -6.890 8.457 1.00 0.00 H ATOM 782 2HG GLU A 55147.148 -8.113 8.362 1.00 0.00 H ATOM 783 N ASPA 56151.713 -9.843 6.385 1.00 0.00 N ATOM 784 CA ASP A 56152.748 -10.852 6.199 1.00 0.00 C ATOM 785 C ASP A 56153.972 -10.256 5.509 1.00 0.00 C ATOM 786 O ASPA 56153.857 -9.318 4.722 1.00 0.00 O ATOM 787 CB ASP A 56152.207 -12.024 5.379 1.00 0.00 C ATOM

788 CG ASPA 56152.759 -13.358 5.842 1.00 0.00 C **ATOM** 789 OD1 ASP A 56152.112 -14.007 6.689 1.00 0.00 O **ATOM** 790 OD2 ASP A 56153.839 -13.754 5.355 1.00 0.00 O **ATOM ATOM** 791 H ASPA 56151.130 -9.612 5.632 1.00 0.00 H **ATOM** 792 HA ASP A 56153.040 -11.212 7.174 1.00 0.00 H **ATOM** 793 1HB ASPA 56151.131 -12.052 5.468 1.00 0.00 H **ATOM** 794 2HB ASP A 56152.474 -11.884 4.341 1.00 0.00 H 795 N GLUA 57155.142 -10.810 5.811 1.00 0.00 N **ATOM** 796 CA GLUA 57156.387 -10.334 5.219 1.00 0.00 C **ATOM ATOM** 797 C GLUA 57156.650 -11.019 3.882 1.00 0.00 C **ATOM** 798 O GLUA 57156.986 -12.203 3.836 1.00 0.00 O **ATOM** 799 CB GLUA 57157.558 -10.584 6.172 1.00 0.00 C 800 CG GLU A 57157.490 -9.760 7.448 1.00 0.00 C **ATOM ATOM** 801 CD GLUA 57158.429 -10.272 8.522 1.00 0.00 C ATOM 802 OE1 GLU A 57159.608 -10.536 8.205 1.00 0.00 O 803 OE2 GLU A 57157.985 -10.409 9.682 1.00 0.00 O **ATOM** 804 H GLUA 57155.169 -11.556 6.445 1.00 0.00 H ATOM ATOM 805 HA GLU A 57156.291 -9.272 5.053 1.00 0.00 H ATOM 806 1HB GLU A 57157.567 -11.629 6.445 1.00 0.00 H 807 2HB GLU A 57158.480 -10.345 5.663 1.00 0.00 H ATOM ATOM 808 1HG GLUA 57157.756 -8.740 7.216 1.00 0.00 H 809 2HG GLU A 57156.480 -9.791 7.828 1.00 0.00 H **ATOM ATOM** 810 N CYS A 58156.495 -10.269 2.797 1.00 0.00 N 811 CA CYS A 58156.716 -10.804 1.459 1.00 0.00 C ATOM **ATOM** 812 C CYS A 58157.997 -10.242 0.851 1.00 0.00 C ATOM 813 O CYS A 58158.317 -9.067 1.030 1.00 0.00 O 814 CB CYS A 58155.524 -10.482 0.554 1.00 0.00 C ATOM 815 SG CYS A 58154.176 -11.683 0.653 1.00 0.00 S **ATOM** 816 H CYS A 58156.226 -9.331 2.898 1.00 0.00 H ATOM ATOM 817 HA CYS A 58156.812 -11.877 1.542 1.00 0.00 H ATOM 818 1HB CYS A 58155.125 -9.517 0.830 1.00 0.00 H

- ATOM 819 2HB CYS A 58155.861 -10.447 -0.472 1.00 0.00 H
- ATOM 820 HG CYS A 58154.554 -12.533 0.888 1.00 0.00 H
- ATOM 821 N ALAA 59158.726 -11.089 0.133 1.00 0.00 N
- ATOM 822 CA ALAA 59159.972 -10.677 -0.502 1.00 0.00 C
- ATOM 823 C ALA A 59159.708 -9.725 -1.664 1.00 0.00 C
- ATOM 824 O ALAA 59159.129 -10.113 -2.678 1.00 0.00 O
- ATOM 825 CB ALAA 59160.747 -11.895 -0.981 1.00 0.00 C
- ATOM 826 H ALAA 59158.418 -12.014 0.026 1.00 0.00 H
- ATOM 827 HA ALA A 59160.570 -10.168 0.239 1.00 0.00 H
- ATOM 828 1HB ALA A 59161.352 -11.625 -1.834 1.00 0.00 H
- ATOM 829 2HB ALA A 59160.054 -12.674 -1.265 1.00 0.00 H
- ATOM 830 3HB ALA A 59161.385 -12.252 -0.186 1.00 0.00 H
- ATOM 831 N GLY A 60160.136 -8.476 -1.508 1.00 0.00 N
- ATOM 832 CA GLY A 60159.937 -7.489 -2.551 1.00 0.00 C
- ATOM 833 C GLY A 60159.402 -6.175 -2.012 1.00 0.00 C
- ATOM 834 O GLY A 60159.649 -5.115 -2.587 1.00 0.00 O
- ATOM 835 H GLY A 60160.591 -8.225 -0.677 1.00 0.00 H
- ATOM 836 1HA GLY A 60160.880 -7.305 -3.044 1.00 0.00 H
- ATOM 837 2HA GLY A 60159.236 -7.880 -3.274 1.00 0.00 H
- ATOM 838 N CYS A 61158.669 -6.247 -0.907 1.00 0.00 N
- ATOM 839 CA CYS A 61158.098 -5.055 -0.290 1.00 0.00 C
- ATOM 840 C CYS A 61159.175 -4.242 0.422 1.00 0.00 C
- ATOM 841 O CYS A 61160.259 -4.749 0.712 1.00 0.00 O
- ATOM 842 CB CYS A 61156.999 -5.444 0.700 1.00 0.00 C
- ATOM 843 SG CYS A 61155.806 -6.635 0.046 1.00 0.00 S
- ATOM 844 H CYS A 61158.508 -7.121 -0.495 1.00 0.00 H
- ATOM 845 HA CYS A 61157.667 -4.450 -1.074 1.00 0.00 H
- ATOM 846 1HB CYS A 61157.452 -5.882 1.576 1.00 0.00 H
- ATOM 847 2HB CYS A 61156.453 -4.556 0.988 1.00 0.00 H
- ATOM 848 HG CYS A 61156.257 -7.181 -0.602 1.00 0.00 H
- ATOM 849 N THR A 62158.869 -2.979 0.700 1.00 0.00 N

- ATOM 850 CA THR A 62159.811 -2.096 1.378 1.00 0.00 C
- ATOM 851 C THR A 62159.450 -1.944 2.852 1.00 0.00 C
- ATOM 852 O THR A 62158.508 -2.571 3.338 1.00 0.00 O
- ATOM 853 CB THR A 62159.834 -0.725 0.702 1.00 0.00 C
- ATOM 854 OG1 THR A 62158.569 -0.422 0.140 1.00 0.00 O
- ATOM 855 CG2 THR A 62160.865 -0.617 -0.400 1.00 0.00 C
- ATOM 856 H THR A 62157.989 -2.632 0.443 1.00 0.00 H
- ATOM 857 HA THR A 62160.793 -2.540 1.305 1.00 0.00 H
- ATOM 858 HB THR A 62160.063 0.027 1.444 1.00 0.00 H
- ATOM 859 HG1 THR A 62158.577 0.476 -0.200 1.00 0.00 H
- ATOM 860 1HG2 THR A 62161.107 0.422 -0.567 1.00 0.00 H
- ATOM 861 2HG2 THR A 62160.466 -1.044 -1.309 1.00 0.00 H
- ATOM 862 3HG2 THR A 62161.757 -1.153 -0.112 1.00 0.00 H
- ATOM 863 N ASPA 63160.204 -1.108 3.557 1.00 0.00 N
- ATOM 864 CA ASP A 63159.963 -0.873 4.977 1.00 0.00 C
- ATOM 865 C ASPA 63159.263 0.463 5.197 1.00 0.00 C
- ATOM 866 O ASPA 63159.501 1.144 6.194 1.00 0.00 O
- ATOM 867 CB ASPA 63161.283 -0.905 5.752 1.00 0.00 C
- ATOM 868 CG ASP A 63162.354 -0.050 5.104 1.00 0.00 C
- ATOM 869 OD1 ASP A 63163.372 -0.615 4.652 1.00 0.00 O
- ATOM 870 OD2 ASP A 63162.175 1.185 5.048 1.00 0.00 O
- ATOM 871 H ASPA 63160.940 -0.637 3.114 1.00 0.00 H
- ATOM 872 HA ASPA 63159.324 -1.665 5.339 1.00 0.00 H
- ATOM 873 1HB ASP A 63161.114 -0.538 6.753 1.00 0.00 H
- ATOM 874 2HB ASP A 63161.640 -1.922 5.800 1.00 0.00 H
- ATOM 875 N GLY A 64158.398 0.833 4.258 1.00 0.00 N
- ATOM 876 CA GLY A 64157.676 2.087 4.367 1.00 0.00 C
- ATOM 877 C GLY A 64158.318 3.199 3.562 1.00 0.00 C
- ATOM 878 O GLY A 64158.413 4.336 4.025 1.00 0.00 O
- ATOM 879 H GLY A 64158.249 0.250 3.485 1.00 0.00 H
- ATOM 880 1HA GLY A 64156.666 1.940 4.016 1.00 0.00 H

881 2HA GLY A 64157.644 2.382 5.406 1.00 0.00 H ATOM 882 N THR A 65158.763 2.871 2.353 1.00 0.00 N **ATOM** 883 CA THR A 65159.400 3.850 1.481 1.00 0.00 C 884 C THR A 65159.035 3.600 0.022 1.00 0.00 C ATOM 885 O THR A 65159.312 2.531 -0.524 1.00 0.00 O ATOM ATOM 886 CB THR A 65160.919 3.805 1.652 1.00 0.00 C ATOM 887 OG1 THR A 65161.395 2.473 1.559 1.00 0.00 O 888 CG2 THR A 65161.390 4.368 2.976 1.00 0.00 C **ATOM** 889 H THR A 65158.659 1.948 2.040 1.00 0.00 H ATOM **ATOM** 890 HA THR A 65159.044 4.829 1.766 1.00 0.00 H ATOM 891 HB THR A 65161.377 4.385 0.865 1.00 0.00 H **ATOM** 892 HG1 THR A 65161.050 2.065 0.762 1.00 0.00 H 893 1HG2 THR A 65160.959 5.348 3.123 1.00 0.00 H ATOM 894 2HG2 THR A 65162.466 4.445 2.972 1.00 0.00 H ATOM 895 3HG2 THR A 65161.078 3.714 3.777 1.00 0.00 H ATOM 896 N PHE A 66158.411 4.591 -0.606 1.00 0.00 N **ATOM** 897 CA PHE A 66158.008 4.479 -2.003 1.00 0.00 C ATOM 898 C PHE A 66159.094 5.022 -2.927 1.00 0.00 C **ATOM** 899 O PHE A 66159.201 6.230 -3.130 1.00 0.00 O ATOM 900 CB PHE A 66156.697 5.230 -2.241 1.00 0.00 C **ATOM** 901 CG PHE A 66156.012 4.848 -3.522 1.00 0.00 C ATOM ATOM 902 CD1 PHE A 66155.529 5.822 -4.381 1.00 0.00 C 903 CD2 PHE A 66155.849 3.516 -3.865 1.00 0.00 C ATOM 904 CE1 PHE A 66154.899 5.474 -5.560 1.00 0.00 C ATOM 905 CE2 PHE A 66155.218 3.161 -5.042 1.00 0.00 C ATOM 906 CZ PHE A 66154.742 4.141 -5.892 1.00 0.00 C ATOM 907 H PHE A 66158.218 5.419 -0.118 1.00 0.00 H ATOM 908 HA PHE A 66157.857 3.432 -2.220 1.00 0.00 H ATOM 909 1HB PHE A 66156.019 5.023 -1.427 1.00 0.00 H ATOM 910 2HB PHE A 66156.900 6.290 -2.274 1.00 0.00 H ATOM ATOM 911 HD1 PHE A 66155.652 6.864 -4.124 1.00 0.00 H

912 HD2 PHE A 66156.220 2.748 -3.202 1.00 0.00 H 913 HE1 PHE A 66154.528 6.242 -6.223 1.00 0.00 H ATOM ATOM 914 HE2 PHE A 66155.098 2.119 -5.299 1.00 0.00 H ATOM 915 HZ PHE A 66154.250 3.867 -6.812 1.00 0.00 H ATOM 916 N ARG A 67159.896 4.119 -3.483 1.00 0.00 N ATOM 917 CA ARG A 67160.973 4.509 -4.386 1.00 0.00 C 918 C ARG A 67161.960 5.438 -3.686 1.00 0.00 C ATOM 919 O ARGA 67162.592 6.281 -4.322 1.00 0.00 O ATOM 920 CB ARG A 67160.404 5.194 -5.629 1.00 0.00 C ATOM ATOM 921 CG ARG A 67159.247 4.438 -6.263 1.00 0.00 C **ATOM** 922 CD ARG A 67158.335 5.371 -7.047 1.00 0.00 C **ATOM** 923 NE ARG A 67158.608 5.327 -8.481 1.00 0.00 N ATOM 924 CZ ARG A 67158.258 4.314 -9.271 1.00 0.00 C ATOM 925 NH1 ARG A 67157.622 3.261 -8.771 1.00 0.00 N ATOM 926 NH2 ARG A 67158.544 4.354 -10.566 1.00 0.00 N 927 H ARGA 67159.759 3.170 -3.282 1.00 0.00 H ATOM 928 HA ARG A 67161.493 3.612 -4.686 1.00 0.00 H ATOM ATOM 929 1HB ARG A 67160.055 6.179 -5.355 1.00 0.00 H ATOM 930 2HB ARG A 67161.188 5.290 -6.365 1.00 0.00 H 931 1HG ARG A 67159.642 3.691 -6.935 1.00 0.00 H **ATOM ATOM** 932 2HG ARG A 67158.673 3.959 -5.484 1.00 0.00 H 933 1HD ARG A 67157.310 5.077 -6.876 1.00 0.00 H ATOM 934 2HD ARG A 67158.483 6.380 -6.691 1.00 0.00 H ATOM ATOM 935 HE ARG A 67159.077 6.091 -8.876 1.00 0.00 H 936 1HH1 ARG A 67157.403 3.225 -7.795 1.00 0.00 H ATOM 937 2HH1 ARG A 67157.361 2.504 -9.370 1.00 0.00 H ATOM ATOM 938 1HH2 ARG A 67159.022 5.145 -10.947 1.00 0.00 H 939 2HH2 ARG A 67158.282 3.594 -11.159 1.00 0.00 H ATOM ATOM 940 N GLY A 68162.086 5.279 -2.372 1.00 0.00 N ATOM 941 CA GLY A 68162.998 6.111 -1.610 1.00 0.00 C ATOM 942 C GLY A 68162.279 7.180 -0.808 1.00 0.00 C

- ATOM 943 O GLY A 68162.795 7.658 0.202 1.00 0.00 O
- ATOM 944 H GLY A 68161.558 4.591 -1.917 1.00 0.00 H
- ATOM 945 1HA GLY A 68163.558 5.485 -0.931 1.00 0.00 H
- ATOM 946 2HA GLY A 68163.686 6.590 -2.291 1.00 0.00 H
- ATOM 947 N THR A 69161.086 7.556 -1.260 1.00 0.00 N
- ATOM 948 CA THR A 69160.299 8.575 -0.576 1.00 0.00 C
- ATOM 949 C THR A 69159.624 8.002 0.666 1.00 0.00 C
- ATOM 950 O THR A 69158.538 7.428 0.585 1.00 0.00 O
- ATOM 951 CB THR A 69159.245 9.152 -1.523 1.00 0.00 C
- ATOM 952 OG1 THR A 69159.760 9.271 -2.836 1.00 0.00 O
- ATOM 953 CG2 THR A 69158.746 10.518 -1.101 1.00 0.00 C
- ATOM 954 H THR A 69160.728 7.138 -2.070 1.00 0.00 H
- ATOM 955 HA THR A 69160.969 9.365 -0.275 1.00 0.00 H
- ATOM 956 HB THR A 69158.396 8.484 -1.549 1.00 0.00 H
- ATOM 957 HG1 THR A 69159.603 8.454 -3.317 1.00 0.00 H
- ATOM 958 1HG2 THR A 69157.684 10.586 -1.285 1.00 0.00 H
- ATOM 959 2HG2 THR A 69159.259 11.280 -1.670 1.00 0.00 H
- ATOM 960 3HG2 THR A 69158.939 10.663 -0.048 1.00 0.00 H
- ATOM 961 N ARG A 70160.275 8.161 1.813 1.00 0.00 N
- ATOM 962 CA ARG A 70159.738 7.659 3.073 1.00 0.00 C
- ATOM 963 C ARG A 70158.513 8.463 3.499 1.00 0.00 C
- ATOM 964 O ARG A 70158.554 9.692 3.554 1.00 0.00 O
- ATOM 965 CB ARG A 70160.806 7.716 4.166 1.00 0.00 C
- ATOM 966 CG ARG A 70160.332 7.181 5.508 1.00 0.00 C
- ATOM 967 CD ARG A 70160.920 7.975 6.663 1.00 0.00 C
- ATOM 968 NE ARG A 70162.233 7.472 7.062 1.00 0.00 N
- ATOM 969 CZ ARG A 70163.084 8.150 7.828 1.00 0.00 C
- ATOM 970 NH1 ARG A 70162.766 9.356 8.281 1.00 0.00 N
- ATOM 971 NH2 ARG A 70164.258 7.619 8.143 1.00 0.00 N
- ATOM 972 H ARG A 70161.137 8.627 1.813 1.00 0.00 H
- ATOM 973 HA ARG A 70159.444 6.631 2.921 1.00 0.00 H

ATOM 974 1HB ARG A 70161.659 7.134 3.851 1.00 0.00 H **ATOM** 975 2HB ARG A 70161.112 8.743 4.300 1.00 0.00 H 976 1HG ARG A 70159.255 7.245 5.551 1.00 0.00 H **ATOM** 977 2HG ARG A 70160.636 6.149 5.600 1.00 0.00 H ATOM 978 1HD ARG A 70161.017 9.007 6.361 1.00 0.00 H **ATOM** ATOM 979 2HD ARG A 70160.248 7.909 7.506 1.00 0.00 H 980 HE ARG A 70162.494 6.584 6.741 1.00 0.00 H ATOM 981 1HH1 ARG A 70161.882 9.762 8.048 1.00 0.00 H **ATOM** 982 2HH1 ARG A 70163.409 9.859 8.857 1.00 0.00 H **ATOM ATOM** 983 1HH2 ARG A 70164.503 6.711 7.805 1.00 0.00 H ATOM 984 2HH2 ARG A 70164.898 8.127 8.720 1.00 0.00 H 985 N TYR A 71157.426 7.760 3.799 1.00 0.00 N ATOM 986 CA TYR A 71156.189 8.408 4.220 1.00 0.00 C ATOM 987 C TYR A 71155.841 8.032 5.657 1.00 0.00 C ATOM 988 O TYR A 71155.425 8.880 6.447 1.00 0.00 O ATOM 989 CB TYR A 71155.042 8.019 3.287 1.00 0.00 C **ATOM** 990 CG TYR A 71155.198 8.551 1.879 1.00 0.00 C ATOM ATOM 991 CD1 TYR A 71155.353 7.686 0.804 1.00 0.00 C 992 CD2 TYR A 71155.192 9.917 1.628 1.00 0.00 C ATOM ATOM 993 CE1 TYR A 71155.496 8.168 -0.485 1.00 0.00 C 994 CE2 TYR A 71155.334 10.406 0.343 1.00 0.00 C **ATOM ATOM** 995 CZ TYR A 71155.486 9.528 -0.709 1.00 0.00 C 996 OH TYR A 71155.628 10.012 -1.989 1.00 0.00 O ATOM 997 H TYR A 71157.456 6.783 3.735 1.00 0.00 H ATOM ATOM 998 HA TYR A 71156.339 9.476 4.167 1.00 0.00 H 999 1HB TYR A 71154.983 6.943 3.229 1.00 0.00 H ATOM ATOM 1000 2HB TYR A 71154.116 8.405 3.687 1.00 0.00 H ATOM 1001 HD1 TYR A 71155.360 6.621 0.982 1.00 0.00 H ATOM 1002 HD2 TYR A 71155.073 10.603 2.454 1.00 0.00 H ATOM 1003 HE1 TYR A 71155.615 7.480 -1.308 1.00 0.00 H ATOM 1004 HE2 TYR A 71155.326 11.472 0.168 1.00 0.00 H

ATOM 1005 HH TYR A 71154.788 10.360 -2.295 1.00 0.00 H ATOM 1006 N PHE A 72156.013 6.757 5.987 1.00 0.00 N ATOM 1007 CA PHE A 72155.716 6.268 7.329 1.00 0.00 C ATOM 1008 C PHE A 72156.781 5.282 7.797 1.00 0.00 C ATOM 1009 O PHE A 72157.740 5.001 7.079 1.00 0.00 O ATOM 1010 CB PHE A 72154.339 5.603 7.358 1.00 0.00 C ATOM 1011 CG PHE A 72154.122 4.623 6.241 1.00 0.00 C ATOM 1012 CD1 PHE A 72154.270 3.261 6.457 1.00 0.00 C ATOM 1013 CD2 PHE A 72153.771 5.062 4.974 1.00 0.00 C ATOM 1014 CE1 PHE A 72154.071 2.357 5.431 1.00 0.00 C ATOM 1015 CE2 PHE A 72153.570 4.163 3.944 1.00 0.00 C ATOM 1016 CZ PHE A 72153.720 2.809 4.173 1.00 0.00 C ATOM 1017 H PHE A 72156.346 6.129 5.313 1.00 0.00 H ATOM 1018 HA PHE A 72155.710 7.117 7.997 1.00 0.00 H ATOM 1019 1HB PHE A 72154.223 5.072 8.291 1.00 0.00 H ATOM 1020 2HB PHE A 72153.578 6.365 7.285 1.00 0.00 H ATOM 1021 HD1 PHE A 72154.543 2.908 7.440 1.00 0.00 H ATOM 1022 HD2 PHE A 72153.653 6.120 4.795 1.00 0.00 H ATOM 1023 HE1 PHE A 72154.190 1.300 5.612 1.00 0.00 H ATOM 1024 HE2 PHE A 72153.297 4.519 2.962 1.00 0.00 H ATOM 1025 HZ PHE A 72153.564 2.104 3.370 1.00 0.00 H ATOM 1026 N THR A 73156.605 4.760 9.007 1.00 0.00 N ATOM 1027 CA THR A 73157.551 3.805 9.573 1.00 0.00 C ATOM 1028 C THR A 73156.871 2.469 9.856 1.00 0.00 C ATOM 1029 O THR A 73156.113 2.338 10.817 1.00 0.00 O ATOM 1030 CB THR A 73158.162 4.361 10.860 1.00 0.00 C ATOM 1031 OG1 THR A 73157.244 5.211 11.525 1.00 0.00 O ATOM 1032 CG2 THR A 73159.432 5.152 10.626 1.00 0.00 C ATOM 1033 H THR A 73155.821 5.023 9.533 1.00 0.00 H ATOM 1034 HA THR A 73158.337 3.648 8.850 1.00 0.00 H ATOM 1035 HB THR A 73158.401 3.539 11.518 1.00 0.00 H

ATOM 1036 HG1 THR A 73156.707 4.692 12.128 1.00 0.00 H ATOM 1037 1HG2 THR A 73159.457 5.998 11.296 1.00 0.00 H ATOM 1038 2HG2 THR A 73159.456 5.500 9.604 1.00 0.00 H ATOM 1039 3HG2 THR A 73160.288 4.521 10.812 1.00 0.00 H ATOM 1040 N CYS A 74157.149 1.479 9.013 1.00 0.00 N ATOM 1041 CA CYS A 74156.565 0.153 9.173 1.00 0.00 C ATOM 1042 C CYS A 74157.648 -0.922 9.171 1.00 0.00 C ATOM 1043 O CYS A 74158.817 -0.639 8.913 1.00 0.00 O ATOM 1044 CB CYS A 74155.556 -0.121 8.056 1.00 0.00 C ATOM 1045 SG CYS A 74153.872 0.415 8.436 1.00 0.00 S ATOM 1046 H CYS A 74157.762 1.645 8.266 1.00 0.00 H ATOM 1047 HA CYS A 74156.052 0.128 10.122 1.00 0.00 H ATOM 1048 1HB CYS A 74155.871 0.396 7.162 1.00 0.00 H ATOM 1049 2HB CYS A 74155.527 -1.183 7.860 1.00 0.00 H ATOM 1050 HG CYS A 74153.370 -0.356 8.709 1.00 0.00 H ATOM 1051 N ALAA 75157.249 -2.157 9.460 1.00 0.00 N ATOM 1052 CA ALA A 75158.185 -3.274 9.491 1.00 0.00 C ATOM 1053 C ALA A 75158.860 -3.461 8.137 1.00 0.00 C ATOM 1054 O ALAA 75158.563 -2.747 7.180 1.00 0.00 O ATOM 1055 CB ALA A 75157.469 -4.549 9.908 1.00 0.00 C ATOM 1056 H ALAA 75156.303 -2.320 9.657 1.00 0.00 H ATOM 1057 HA ALA A 75158.940 -3.054 10.232 1.00 0.00 H ATOM 1058 1HB ALAA 75156.425 -4.479 9.643 1.00 0.00 H ATOM 1059 2HB ALA A 75157.562 -4.681 10.976 1.00 0.00 H ATOM 1060 3HB ALA A 75157.913 -5.393 9.401 1.00 0.00 H ATOM 1061 N LEU A 76159.770 -4.427 8.064 1.00 0.00 N ATOM 1062 CA LEU A 76160.488 -4.709 6.827 1.00 0.00 C ATOM 1063 C LEUA 76159.705 -5.684 5.953 1.00 0.00 C ATOM 1064 O LEUA 76159.141 -6.660 6.447 1.00 0.00 O ATOM 1065 CB LEU A 76161.873 -5.281 7.135 1.00 0.00 C ATOM 1066 CG LEU A 76162.966 -4.238 7.375 1.00 0.00 C

ATOM 1067 CD1 LEU A 76164.095 -4.830 8,205 1.00 0.00 C ATOM 1068 CD2 LEU A 76163.495 -3.708 6.051 1.00 0.00 C ATOM 1069 H LEUA 76159.964 -4.963 8.862 1.00 0.00 H ATOM 1070 HA LEU A 76160.604 -3.778 6.292 1.00 0.00 H ATOM 1071 1HB LEU A 76161.795 -5.901 8.016 1.00 0.00 H ATOM 1072 2HB LEU A 76162.176 -5.901 6.305 1.00 0.00 H ATOM 1073 HG LEU A 76162.547 -3.408 7.926 1.00 0.00 H ATOM 1074 1HD1 LEU A 76164.504 -4.068 8.851 1.00 0.00 H ATOM 1075 2HD1 LEU A 76164.869 -5.199 7.548 1.00 0.00 H ATOM 1076 3HD1 LEU A 76163.713 -5.643 8.803 1.00 0.00 H ATOM 1077 1HD2 LEU A 76163.973 -2.752 6.212 1.00 0.00 H ATOM 1078 2HD2 LEU A 76162.676 -3.589 5.357 1.00 0.00 H ATOM 1079 3HD2 LEU A 76164.213 -4.406 5.645 1.00 0.00 H ATOM 1080 N LYS A 77159.676 -5.413 4.652 1.00 0.00 N ATOM 1081 CA LYS A 77158.962 -6.266 3.709 1.00 0.00 C ATOM 1082 C LYS A 77157.473 -6.313 4.036 1.00 0.00 C ATOM 1083 O LYS A 77156.840 -7.365 3.949 1.00 0.00 O ATOM 1084 CB LYS A 77159.546 -7.681 3.727 1.00 0.00 C ATOM 1085 CG LYS A 77161.022 -7.735 3.366 1.00 0.00 C ATOM 1086 CD LYS A 77161.222 -7.948 1.874 1.00 0.00 C ATOM 1087 CE LYS A 77162.466 -7.232 1.372 1.00 0.00 C ATOM 1088 NZ LYS A 77163.176 -8.018 0.325 1.00 0.00 N ATOM 1089 H LYS A 77160.145 -4.620 4.319 1.00 0.00 H ATOM 1090 HA LYS A 77159.089 -5.848 2.722 1.00 0.00 H ATOM 1091 1HB LYS A 77159.425 -8.095 4.717 1.00 0.00 H ATOM 1092 2HB LYS A 77159.002 -8.292 3.022 1.00 0.00 H ATOM 1093 1HG LYS A 77161.487 -6.804 3.653 1.00 0.00 H ATOM 1094 2HG LYS A 77161.484 -8.552 3.902 1.00 0.00 H ATOM 1095 1HD LYS A 77161.325 -9.005 1.681 1.00 0.00 H ATOM 1096 2HD LYS A 77160.360 -7.566 1.347 1.00 0.00 H ATOM 1097 1HE LYS A 77162.174 -6.278 0.956 1.00 0.00 H

ATOM 1098 2HE LYS A 77163.133 -7.070 2.205 1.00 0.00 H ATOM 1099 1HZ LYS A 77162.881 -7.702 -0.620 1.00 0.00 H ATOM 1100 2HZ LYS A 77162,953 -9.029 0.426 1.00 0.00 H ATOM 1101 3HZ LYS A 77164.204 -7.890 0.418 1.00 0.00 H ATOM 1102 N LYS A 78156.919 -5.165 4.412 1.00 0.00 N ATOM 1103 CA LYS A 78155.503 -5.075 4.751 1.00 0.00 C ATOM 1104 C LYS A 78154.937 -3.711 4.366 1.00 0.00 C ATOM 1105 O LYS A 78154.084 -3.163 5.064 1.00 0.00 O ATOM 1106 CB LYS A 78155.299 -5.322 6.246 1.00 0.00 C ATOM 1107 CG LYS A 78155.835 -6.663 6.719 1.00 0.00 C ATOM 1108 CD LYS A 78155.588 -6.870 8.205 1.00 0.00 C ATOM 1109 CE LYS A 78154.371 -7.748 8.450 1.00 0.00 C ATOM 1110 NZ LYS A 78153.592 -7.299 9.636 1.00 0.00 N ATOM 1111 H LYS A 78157.475 -4.359 4.462 1.00 0.00 H ATOM 1112 HA LYS A 78154.980 -5.838 4.193 1.00 0.00 H ATOM 1113 1HB LYS A 78155.801 -4.543 6.800 1.00 0.00 H ATOM 1114 2HB LYS A 78154.242 -5.284 6.464 1.00 0.00 H ATOM 1115 1HG LYS A 78155.342 -7.451 6.169 1.00 0.00 H ATOM 1116 2HG LYS A 78156.898 -6.702 6.531 1.00 0.00 H ATOM 1117 1HD LYS A 78156.454 -7.342 8.641 1.00 0.00 H ATOM 1118 2HD LYS A 78155.426 -5.908 8.669 1.00 0.00 H ATOM 1119 1HE LYS A 78153.736 -7.712 7.578 1.00 0.00 H ATOM 1120 2HE LYS A 78154.703 -8.764 8.611 1.00 0.00 H ATOM 1121 1HZ LYS A 78154.204 -6.763 10.284 1.00 0.00 H ATOM 1122 2HZ LYS A 78153.207 -8.121 10.144 1.00 0.00 H ATOM 1123 3HZ LYS A 78152.803 -6.691 9.336 1.00 0.00 H ATOM 1124 N ALA A 79155.417 -3.170 3.252 1.00 0.00 N ATOM 1125 CA ALA A 79154.959 -1.871 2.774 1.00 0.00 C ATOM 1126 C ALA A 79154.768 -1.878 1.261 1.00 0.00 C ATOM 1127 O ALAA 79155.729 -1.743 0.504 1.00 0.00 O ATOM 1128 CB ALA A 79155.942 -0.784 3.179 1.00 0.00 C

ATOM 1129 H ALAA 79156.096 -3.655 2.738 1.00 0.00 H ATOM 1130 HA ALA A 79154.010 -1.659 3.246 1.00 0.00 H ATOM 1131 1HB ALA A 79155.400 0.113 3.442 1.00 0.00 H ATOM 1132 2HB ALA A 79156.607 -0.573 2.354 1.00 0.00 H ATOM 1133 3HB ALAA 79156.519 -1.117 4.028 1.00 0.00 H ATOM 1134 N LEUA 80153.522 -2.038 0.829 1.00 0.00 N ATOM 1135 CA LEU A 80153.204 -2.063 -0.595 1.00 0.00 C ATOM 1136 C LEU A 80152.375 -0.846 -0.989 1.00 0.00 C ATOM 1137 O LEUA 80151.319 -0.587 -0.410 1.00 0.00 O ATOM 1138 CB LEU A 80152.448 -3.345 -0.947 1.00 0.00 C ATOM 1139 CG LEU A 80152.015 -3.461 -2.409 1.00 0.00 C ATOM 1140 CD1 LEU A 80153.127 -4.072 -3.247 1.00 0.00 C ATOM 1141 CD2 LEU A 80150.742 -4.287 -2.524 1.00 0.00 C ATOM 1142 H LEUA 80152.798 -2.140 1.481 1.00 0.00 H ATOM 1143 HA LEU A 80154.135 -2.042 -1.143 1.00 0.00 H ATOM 1144 1HB LEU A 80153.083 -4.188 -0.712 1.00 0.00 H ATOM 1145 2HB LEU A 80151.565 -3.399 -0.328 1.00 0.00 H ATOM 1146 HG LEU A 80151.811 -2.473 -2.795 1.00 0.00 H ATOM 1147 1HD1 LEU A 80153.127 -3.621 -4.229 1.00 0.00 H ATOM 1148 2HD1 LEU A 80152.964 -5.136 -3.340 1.00 0.00 H ATOM 1149 3HD1 LEU A 80154.078 -3.894 -2.769 1.00 0.00 H ATOM 1150 1HD2 LEU A 80150.387 -4.261 -3.543 1.00 0.00 H ATOM 1151 2HD2 LEU A 80149.988 -3.878 -1.868 1.00 0.00 H ATOM 1152 3HD2 LEU A 80150.950 -5.308 -2.240 1.00 0.00 H ATOM 1153 N PHE A 81152.859 -0.100 -1.976 1.00 0.00 N ATOM 1154 CA PHE A 81152.162 1.091 -2.449 1.00 0.00 C ATOM 1155 C PHE A 81151.323 0.776 -3.683 1.00 0.00 C ATOM 1156 O PHE A 81151.796 0.136 -4.621 1.00 0.00 O ATOM 1157 CB PHE A 81153.164 2.201 -2.768 1.00 0.00 C ATOM 1158 CG PHE A 81153.781 2.823 -1.548 1.00 0.00 C ATOM 1159 CD1 PHE A 81154.882 2.242 -0.940 1.00 0.00 C

ATOM 1160 CD2 PHE A 81153.260 3.988 -1.009 1.00 0.00 C ATOM 1161 CE1 PHE A 81155.453 2.812 0.182 1.00 0.00 C ATOM 1162 CE2 PHE A 81153.826 4.563 0.113 1.00 0.00 C ATOM 1163 CZ PHE A 81154.924 3.973 0.710 1.00 0.00 C ATOM 1164 H PHE A 81153.705 -0.357 -2.399 1.00 0.00 H ATOM 1165 HA PHE A 81151.507 1.426 -1.658 1.00 0.00 H ATOM 1166 1HB PHE A 81153.961 1.794 -3.372 1.00 0.00 H ATOM 1167 2HB PHE A 81152.662 2.981 -3.323 1.00 0.00 H ATOM 1168 HD1 PHE A 81155.297 1.334 -1.352 1.00 0.00 H ATOM 1169 HD2 PHE A 81152.401 4.449 -1.475 1.00 0.00 H ATOM 1170 HE1 PHE A 81156.311 2.349 0.646 1.00 0.00 H ATOM 1171 HE2 PHE A 81153.410 5.471 0.523 1.00 0.00 H ATOM 1172 HZ PHE A 81155.368 4.421 1.586 1.00 0.00 H ATOM 1173 N VALA 82150.074 1.230 -3.674 1.00 0.00 N ATOM 1174 CA VALA 82149.168 0.997 -4.793 1.00 0.00 C ATOM 1175 C VALA 82148.207 2.167 -4.975 1.00 0.00 C ATOM 1176 O VALA 82148.090 3.029 -4.105 1.00 0.00 O ATOM 1177 CB VALA 82148.354 -0.295 -4.597 1.00 0.00 C ATOM 1178 CG1 VAL A 82149.264 -1.512 -4.631 1.00 0.00 C ATOM 1179 CG2 VAL A 82147.570 -0.241 -3.294 1.00 0.00 C ATOM 1180 H VALA 82149.753 1.734 -2.896 1.00 0.00 H ATOM 1181 HA VALA 82149.764 0.890 -5.687 1.00 0.00 H ATOM 1182 HB VALA 82147.648 -0.379 -5.412 1.00 0.00 H ATOM 1183 1HG1 VAL A 82150.134 -1.294 -5.233 1.00 0.00 H ATOM 1184 2HG1 VAL A 82148.732 -2.349 -5.058 1.00 0.00 H ATOM 1185 3HG1 VAL A 82149.574 -1.758 -3.626 1.00 0.00 H ATOM 1186 1HG2 VAL A 82147.581 -1.214 -2.825 1.00 0.00 H ATOM 1187 2HG2 VAL A 82146.551 0.050 -3.498 1.00 0.00 H ATOM 1188 3HG2 VAL A 82148.025 0.482 -2.631 1.00 0.00 H ATOM 1189 N LYS A 83147.522 2.190 -6.114 1.00 0.00 N ATOM 1190 CA LYS A 83146.571 3.255 -6.413 1.00 0.00 C

ATOM 1191 C LYS A 83145.380 3.204 -5.464 1.00 0.00 C ATOM 1192 O LYS A 83144.707 2.180 -5.348 1.00 0.00 O ATOM 1193 CB LYS A 83146.091 3.145 -7.860 1.00 0.00 C ATOM 1194 CG LYS A 83147.213 3.230 -8.882 1.00 0.00 C ATOM 1195 CD LYS A 83146.736 2.827 -10.268 1.00 0.00 C ATOM 1196 CE LYS A 83147.304 3.741 -11.341 1.00 0.00 C ATOM 1197 NZ LYS A 83147.522 3.022 -12.627 1.00 0.00 N ATOM 1198 H LYS A 83147.660 1.475 -6.769 1.00 0.00 H ATOM 1199 HA LYS A 83147.079 4.199 -6.281 1.00 0.00 H ATOM 1200 1HB LYS A 83145.586 2.200 -7.989 1.00 0.00 H ATOM 1201 2HB LYS A 83145.393 3.945 -8.058 1.00 0.00 H ATOM 1202 1HG LYS A 83147.577 4.246 -8.918 1.00 0.00 H ATOM 1203 2HG LYS A 83148.012 2.569 -8.579 1.00 0.00 H ATOM 1204 1HD LYS A 83147.055 1.814 -10.467 1.00 0.00 H ATOM 1205 2HD LYS A 83145.658 2.878 -10.297 1.00 0.00 H ATOM 1206 1HE LYS A 83146.613 4.554 -11.507 1.00 0.00 H ATOM 1207 2HE LYS A 83148.247 4.137 -10.995 1.00 0.00 H ATOM 1208 1HZ LYS A 83148.420 2.497 -12.595 1.00 0.00 H ATOM 1209 2HZ LYS A 83147.557 3.699 -13.414 1.00 0.00 H ATOM 1210 3HZ LYS A 83146.746 2.349 -12.796 1.00 0.00 H ATOM 1211 N LEUA 84145.125 4.318 -4.788 1.00 0.00 N ATOM 1212 CA LEU A 84144.015 4.410 -3.849 1.00 0.00 C ATOM 1213 C LEUA 84142.685 4.149 -4.549 1.00 0.00 C ATOM 1214 O LEUA 84141.743 3.636 -3.944 1.00 0.00 O ATOM 1215 CB LEU A 84143.997 5.791 -3.189 1.00 0.00 C ATOM 1216 CG LEU A 84142.811 6.051 -2.258 1.00 0.00 C ATOM 1217 CD1 LEU A 84142.917 5.194 -1.006 1.00 0.00 C ATOM 1218 CD2 LEU A 84142.737 7.526 -1.891 1.00 0.00 C ATOM 1219 H LEUA 84145.698 5.101 -4.926 1.00 0.00 H ATOM 1220 HA LEU A 84144.162 3.659 -3.087 1.00 0.00 H ATOM 1221 1HB LEU A 84144.908 5.907 -2.620 1.00 0.00 H

ATOM 1222 2HB LEU A 84143.984 6.537 -3.969 1.00 0.00 H ATOM 1223 HG LEU A 84141.896 5.786 -2.767 1.00 0.00 H ATOM 1224 1HD1 LEU A 84143.435 5.745 -0.236 1.00 0.00 H ATOM 1225 2HD1 LEU A 84143.465 4.291 -1.234 1.00 0.00 H ATOM 1226 3HD1 LEU A 84141.927 4.936 -0.662 1.00 0.00 H ATOM 1227 1HD2 LEU A 84141.795 7.729 -1.404 1.00 0.00 H ATOM 1228 2HD2 LEU A 84142.815 8.124 -2.787 1.00 0.00 H ATOM 1229 3HD2 LEU A 84143.549 7.772 -1.222 1.00 0.00 H ATOM 1230 N LYS A 85142.616 4.505 -5.827 1.00 0.00 N ATOM 1231 CA LYS A 85141.401 4.310 -6.611 1.00 0.00 C ATOM 1232 C LYS A 85141.072 2.826 -6.754 1.00 0.00 C ATOM 1233 O LYS A 85139.912 2.453 -6.932 1.00 0.00 O ATOM 1234 CB LYS A 85141.555 4.944 -7.994 1.00 0.00 C ATOM 1235 CG LYS A 85142.656 4.315 -8.833 1.00 0.00 C ATOM 1236 CD LYS A 85143.327 5.341 -9.732 1.00 0.00 C ATOM 1237 CE LYS A 85142.637 5.432 -11.083 1.00 0.00 C ATOM 1238 NZ LYS A 85141.191 5.755 -10.950 1.00 0.00 N ATOM 1239 H LYS A 85143.400 4.910 -6.254 1.00 0.00 H ATOM 1240 HA LYS A 85140.590 4.797 -6.091 1.00 0.00 H ATOM 1241 1HB LYS A 85140.622 4.844 -8.529 1.00 0.00 H ATOM 1242 2HB LYS A 85141.779 5.994 -7.874 1.00 0.00 H ATOM 1243 1HG LYS A 85143.397 3.888 -8.175 1.00 0.00 H ATOM 1244 2HG LYS A 85142.226 3.537 -9.447 1.00 0.00 H ATOM 1245 1HD LYS A 85143.284 6.308 -9.252 1.00 0.00 H ATOM 1246 2HD LYS A 85144.358 5.055 -9.881 1.00 0.00 H ATOM 1247 1HE LYS A 85143.117 6.205 -11.666 1.00 0.00 H ATOM 1248 2HE LYS A 85142.741 4.484 -11.590 1.00 0.00 H ATOM 1249 1HZ LYS A 85140.781 5.957 -11.884 1.00 0.00 H ATOM 1250 2HZ LYS A 85141.065 6.590 -10.342 1.00 0.00 H ATOM 1251 3HZ LYS A 85140.683 4.953 -10.526 1.00 0.00 H ATOM 1252 N SER A 86142.098 1.984 -6.674 1.00 0.00 N

ATOM 1253 CA SER A 86141.913 0.542 -6,794 1.00 0.00 C ATOM 1254 C SER A 86141.835 -0.115 -5.420 1.00 0.00 C ATOM 1255 O SER A 86142.239 -1.265 -5.247 1.00 0.00 O ATOM 1256 CB SER A 86143.057 -0.073 -7.602 1.00 0.00 C ATOM 1257 OG SER A 86143.348 0.704 -8.751 1.00 0.00 O ATOM 1258 H SER A 86143.000 2.340 -6.531 1.00 0.00 H ATOM 1259 HA SER A 86140.984 0.370 -7.316 1.00 0.00 H ATOM 1260 1HB SER A 86143.942 -0.126 -6.986 1.00 0.00 H ATOM 1261 2HB SER A 86142.778 -1.068 -7.916 1.00 0.00 H ATOM 1262 HG SER A 86144.296 0.706 -8.905 1.00 0.00 H ATOM 1263 N CYS A 87141.311 0.621 -4.445 1.00 0.00 N ATOM 1264 CA CYS A 87141.180 0.107 -3.086 1.00 0.00 C ATOM 1265 C CYS A 87139.712 0.006 -2.683 1.00 0.00 C ATOM 1266 O CYS A 87138.868 0.749 -3.182 1.00 0.00 O ATOM 1267 CB CYS A 87141.929 1.008 -2.104 1.00 0.00 C ATOM 1268 SG CYS A 87143.720 1.039 -2.349 1.00 0.00 S ATOM 1269 H CYS A 87141.005 1.530 -4.642 1.00 0.00 H ATOM 1270 HA CYS A 87141.616 -0.880 -3.061 1.00 0.00 H ATOM 1271 1HB CYS A 87141.568 2.020 -2.207 1.00 0.00 H ATOM 1272 2HB CYS A 87141.741 0.665 -1.096 1.00 0.00 H ATOM 1273 HG CYS A 87144.138 0.829 -1.511 1.00 0.00 H ATOM 1274 N ARG A 88139.416 -0.921 -1.777 1.00 0.00 N ATOM 1275 CA ARG A 88138.050 -1.121 -1.307 1.00 0.00 C ATOM 1276 C ARG A 88138.005 -1.203 0.219 1.00 0.00 C ATOM 1277 O ARG A 88138.924 -1.729 0.846 1.00 0.00 O ATOM 1278 CB ARG A 88137.458 -2.394 -1.918 1.00 0.00 C ATOM 1279 CG ARG A 88136.431 -2.125 -3.009 1.00 0.00 C ATOM 1280 CD ARG A 88135.076 -2.726 -2.667 1.00 0.00 C ATOM 1281 NE ARG A 88134.097 -1.701 -2.312 1.00 0.00 N ATOM 1282 CZ ARG A 88133.646 -0.781 -3.162 1.00 0.00 C ATOM 1283 NH1 ARG A 88134.084 -0.752 -4.414 1.00 0.00 N

ATOM 1284 NH2 ARG A 88132.754 0.114 -2.758 1.00 0.00 N ATOM 1285 H ARG A 88140.132 -1.484 -1.416 1.00 0.00 H ATOM 1286 HA ARG A 88137.463 -0.273 -1.627 1.00 0.00 H ATOM 1287 1HB ARG A 88138.260 -2.978 -2.346 1.00 0.00 H ATOM 1288 2HB ARG A 88136.983 -2.969 -1.138 1.00 0.00 H ATOM 1289 1HG ARG A 88136.320 -1.057 -3.128 1.00 0.00 H ATOM 1290 2HG ARG A 88136.784 -2.557 -3.934 1.00 0.00 H ATOM 1291 1HD ARG A 88134.714 -3.274 -3.524 1.00 0.00 H ATOM 1292 2HD ARG A 88135.195 -3.401 -1.832 1.00 0.00 H ATOM 1293 HE ARG A 88133.756 -1.699 -1.393 1.00 0.00 H ATOM 1294 1HH1 ARG A 88134.757 -1.424 -4.726 1.00 0.00 H ATOM 1295 2HH1 ARG A 88133.742 -0.058 -5.047 1.00 0.00 H ATOM 1296 1HH2 ARG A 88132.420 0.097 -1.815 1.00 0.00 H ATOM 1297 2HH2 ARG A 88132.416 0.806 -3.395 1.00 0.00 H ATOM 1298 N PRO A 89136.930 -0.683 0.838 1.00 0.00 N ATOM 1299 CA PRO A 89136.774 -0.703 2.296 1.00 0.00 C ATOM 1300 C PRO A 89136.931 -2.105 2.875 1.00 0.00 C ATOM 1301 O PRO A 89136.144 -3.003 2.574 1.00 0.00 O ATOM 1302 CB PRO A 89135.347 -0.195 2.512 1.00 0.00 C ATOM 1303 CG PRO A 89135.044 0.615 1.300 1.00 0.00 C ATOM 1304 CD PRO A 89135.786 -0.038 0.168 1.00 0.00 C ATOM 1305 HA PRO A 89137.475 -0.037 2.777 1.00 0.00 H ATOM 1306 1HB PRO A 89134.675 -1.035 2.605 1.00 0.00 H ATOM 1307 2HB PRO A 89135.308 0.406 3.408 1.00 0.00 H ATOM 1308 1HG PRO A 89133.981 0.605 1.108 1.00 0.00 H ATOM 1309 2HG PRO A 89135.391 1.628 1.439 1.00 0.00 H ATOM 1310 1HD PRO A 89135.160 -0.772 -0.319 1.00 0.00 H ATOM 1311 2HD PRO A 89136.122 0.703 -0.541 1.00 0.00 H ATOM 1312 N ASPA 90137.951 -2.286 3.707 1.00 0.00 N ATOM 1313 CA ASP A 90138.210 -3.579 4.329 1.00 0.00 C ATOM 1314 C ASP A 90137.750 -3.586 5.783 1.00 0.00 C

ATOM 1315 O ASPA 90138.340 -2.918 6.633 1.00 0.00 O ATOM 1316 CB ASP A 90139.699 -3.915 4.251 1.00 0.00 C ATOM 1317 CG ASP A 90139.952 -5.409 4.179 1.00 0.00 C ATOM 1318 OD1 ASP A 90140.458 -5.974 5.171 1.00 0.00 O ATOM 1319 OD2 ASP A 90139.643 -6.013 3.131 1.00 0.00 O ATOM 1320 H ASPA 90138.543 -1.532 3.909 1.00 0.00 H ATOM 1321 HA ASP A 90137.652 -4.326 3.784 1.00 0.00 H ATOM 1322 1HB ASP A 90140.121 -3.455 3.370 1.00 0.00 H ATOM 1323 2HB ASP A 90140.195 -3.527 5.128 1.00 0.00 H ATOM 1324 N SER A 91136.697 -4.345 6.063 1.00 0.00 N ATOM 1325 CA SER A 91136.163 -4.439 7.417 1.00 0.00 C ATOM 1326 C SER A 91136.405 -5.826 8.004 1.00 0.00 C ATOM 1327 O SER A 91135.654 -6.286 8.864 1.00 0.00 O ATOM 1328 CB SER A 91134.664 -4.130 7.419 1.00 0.00 C ATOM 1329 OG SER A 91134.264 -3.549 8.648 1.00 0.00 O ATOM 1330 H SER A 91136.270 -4.856 5.344 1.00 0.00 H ATOM 1331 HA SER A 91136.672 -3.708 8.027 1.00 0.00 H ATOM 1332 1HB SER A 91134.440 -3.440 6.619 1.00 0.00 H ATOM 1333 2HB SER A 91134.111 -5.046 7.272 1.00 0.00 H ATOM 1334 HG SER A 91134.508 -2.620 8.658 1.00 0.00 H ATOM 1335 N ARG A 92137.459 -6.487 7.536 1.00 0.00 N ATOM 1336 CA ARG A 92137.799 -7.821 8.017 1.00 0.00 C ATOM 1337 C ARG A 92138.193 -7.782 9.490 1.00 0.00 C ATOM 1338 O ARG A 92137.991 -8.751 10.223 1.00 0.00 O ATOM 1339 CB ARG A 92138,940 -8.410 7.187 1.00 0.00 C ATOM 1340 CG ARG A 92138.468 -9.193 5.972 1.00 0.00 C ATOM 1341 CD ARG A 92138.300 -8.294 4.757 1.00 0.00 C ATOM 1342 NE ARG A 92136.945 -8.354 4.214 1.00 0.00 N ATOM 1343 CZ ARG A 92136.620 -7.964 2.984 1.00 0.00 C ATOM 1344 NH1 ARG A 92137.549 -7.484 2.165 1.00 0.00 N ATOM 1345 NH2 ARG A 92135.364 -8.053 2.569 1.00 0.00 N

ATOM 1346 H ARG A 92138.021 -6.068 6.851 1.00 0.00 H ATOM 1347 HA ARG A 92136,925 -8.445 7,907 1.00 0.00 H ATOM 1348 1HB ARG A 92139.575 -7.605 6.845 1.00 0.00 H ATOM 1349 2HB ARG A 92139.520 -9.073 7.812 1.00 0.00 H ATOM 1350 1HG ARG A 92139.195 -9.958 5.744 1.00 0.00 H ATOM 1351 2HG ARG A 92137.518 -9.654 6.201 1.00 0.00 H ATOM 1352 1HD ARG A 92138.517 -7.276 5.043 1.00 0.00 H ATOM 1353 2HD ARG A 92138.997 -8.609 3.994 1.00 0.00 H ATOM 1354 HE ARG A 92136.240 -8.704 4.798 1.00 0.00 H ATOM 1355 1HH1 ARG A 92138.499 -7.414 2.472 1.00 0.00 H ATOM 1356 2HH1 ARG A 92137.299 -7.193 1.242 1.00 0.00 H ATOM 1357 1HH2 ARG A 92134.660 -8.414 3.182 1.00 0.00 H ATOM 1358 2HH2 ARG A 92135.120 -7.759 1.646 1.00 0.00 H ATOM 1359 N PHE A 93138.757 -6.657 9.917 1.00 0.00 N ATOM 1360 CA PHE A 93139.180 -6.492 11.304 1.00 0.00 C ATOM 1361 C PHE A 93138.401 -5.369 11.982 1.00 0.00 C ATOM 1362 O PHE A 93138.910 -4.705 12.885 1.00 0.00 O ATOM 1363 CB PHE A 93140.679 -6.198 11.369 1.00 0.00 C ATOM 1364 CG PHE A 93141.523 -7.226 10.669 1.00 0.00 C ATOM 1365 CD1 PHE A 93142.351 -8.069 11.393 1.00 0.00 C ATOM 1366 CD2 PHE A 93141.487 -7.347 9.290 1.00 0.00 C ATOM 1367 CE1 PHE A 93143.128 -9.015 10.752 1.00 0.00 C ATOM 1368 CE2 PHE A 93142,262 -8,291 8,643 1,00 0,00 C ATOM 1369 CZ PHE A 93143.084 -9.127 9.375 1.00 0.00 C ATOM 1370 H PHE A 93138.892 -5.919 9.286 1.00 0.00 H ATOM 1371 HA PHE A 93138.980 -7.417 11.823 1.00 0.00 H ATOM 1372 1HB PHE A 93140.872 -5.241 10.908 1.00 0.00 H ATOM 1373 2HB PHE A 93140.986 -6.162 12.404 1.00 0.00 H ATOM 1374 HD1 PHE A 93142.386 -7.983 12.469 1.00 0.00 H ATOM 1375 HD2 PHE A 93140.845 -6.695 8.717 1.00 0.00 H ATOM 1376 HE1 PHE A 93143.770 -9.667 11.326 1.00 0.00 H

ATOM 1377 HE2 PHE A 93142,225 -8,376 7,567 1,00 0,00 H ATOM 1378 HZ PHE A 93143.690 -9.865 8.873 1.00 0.00 H ATOM 1379 N ALAA 94137.162 -5.162 11.543 1.00 0.00 N ATOM 1380 CA ALA A 94136.315 -4.119 12.109 1.00 0.00 C ATOM 1381 C ALAA 94136.137 -4.315 13.612 1.00 0.00 C ATOM 1382 O ALA A 94135.661 -5.358 14.061 1.00 0.00 O ATOM 1383 CB ALA A 94134.964 -4.101 11.410 1.00 0.00 C ATOM 1384 H ALAA 94136.811 -5.723 10.819 1.00 0.00 H ATOM 1385 HA ALA A 94136.796 -3.168 11.936 1.00 0.00 H ATOM 1386 1HB ALA A 94134.900 -3.232 10.773 1.00 0.00 H ATOM 1387 2HB ALA A 94134.175 -4.065 12.147 1.00 0.00 H ATOM 1388 3HB ALA A 94134.856 -4.994 10.812 1.00 0.00 H ATOM 1389 N SER A 95136.521 -3.304 14.385 1.00 0.00 N ATOM 1390 CA SER A 95136.403 -3.364 15.837 1.00 0.00 C ATOM 1391 C SER A 95134.940 -3.417 16.263 1.00 0.00 C ATOM 1392 O SER A 95134.056 -2.942 15.549 1.00 0.00 O ATOM 1393 CB SER A 95137.088 -2.155 16.476 1.00 0.00 C ATOM 1394 OG SER A 95138.479 -2.154 16.204 1.00 0.00 O ATOM 1395 H SER A 95136.892 -2.498 13.968 1.00 0.00 H ATOM 1396 HA SER A 95136.895 -4.265 16.172 1.00 0.00 H ATOM 1397 1HB SER A 95136.657 -1.249 16.081 1.00 0.00 H ATOM 1398 2HB SER A 95136.943 -2.187 17.546 1.00 0.00 H ATOM 1399 HG SER A 95138.947 -2.573 16.930 1.00 0.00 H ATOM 1400 N LEU A 96134.689 -3.999 17.432 1.00 0.00 N ATOM 1401 CA LEU A 96133.333 -4.114 17.954 1.00 0.00 C ATOM 1402 C LEUA 96132.453 -4.926 17.010 1.00 0.00 C ATOM 1403 O LEUA 96131.929 -4.402 16.027 1.00 0.00 O ATOM 1404 CB LEU A 96132.727 -2.726 18.167 1.00 0.00 C ATOM 1405 CG LEU A 96131.527 -2.680 19.115 1.00 0.00 C ATOM 1406 CD1 LEU A 96131.490 -1.359 19.866 1.00 0.00 C ATOM 1407 CD2 LEU A 96130.232 -2.895 18.344 1.00 0.00 C

ATOM 1408 H LEU A 96135.436 -4.359 17.956 1.00 0.00 H ATOM 1409 HA LEU A 96133.386 -4.624 18.904 1.00 0.00 H ATOM 1410 1HB LEU A 96133.496 -2.077 18.561 1.00 0.00 H ATOM 1411 2HB LEU A 96132.413 -2.342 17.208 1.00 0.00 H ATOM 1412 HG LEU A 96131.621 -3.475 19.840 1.00 0.00 H ATOM 1413 1HD1 LEU A 96131.103 -0.587 19.218 1.00 0.00 H ATOM 1414 2HD1 LEU A 96132.487 -1.097 20.183 1.00 0.00 H ATOM 1415 3HD1 LEU A 96130.851 -1.456 20.732 1.00 0.00 H ATOM 1416 1HD2 LEU A 96130.444 -3.422 17.426 1.00 0.00 H ATOM 1417 2HD2 LEU A 96129.787 -1.938 18.116 1.00 0.00 H ATOM 1418 3HD2 LEU A 96129.548 -3.477 18.945 1.00 0.00 H ATOM 1419 N GLN A 97132.295 -6.211 17.314 1.00 0.00 N ATOM 1420 CA GLN A 97131.478 -7.096 16.492 1.00 0.00 C ATOM 1421 C GLN A 97130.853 -8.204 17.339 1.00 0.00 C ATOM 1422 O GLN A 97131.005 -9.388 17.040 1.00 0.00 O ATOM 1423 CB GLN A 97132.321 -7.708 15.371 1.00 0.00 C ATOM 1424 CG GLN A 97131.511 -8.109 14.149 1.00 0.00 C ATOM 1425 CD GLN A 97132.049 -9.356 13.476 1.00 0.00 C ATOM 1426 OE1 GLN A 97132.386 -10.337 14.138 1.00 0.00 O ATOM 1427 NE2 GLN A 97132.134 -9.323 12.151 1.00 0.00 N ATOM 1428 H GLN A 97132.738 -6.571 18.110 1.00 0.00 H ATOM 1429 HA GLN A 97130.687 -6.506 16.055 1.00 0.00 H ATOM 1430 1HB GLN A 97133.065 -6.987 15.061 1.00 0.00 H ATOM 1431 2HB GLN A 97132.821 -8.588 15.750 1.00 0.00 H ATOM 1432 1HG GLN A 97130.492 -8.296 14.455 1.00 0.00 H ATOM 1433 2HG GLN A 97131.530 -7.296 13.438 1.00 0.00 H ATOM 1434 1HE2 GLN A 97131.847 -8.508 11.689 1.00 0.00 H ATOM 1435 2HE2 GLN A 97132.478 -10.116 11.690 1.00 0.00 H ATOM 1436 N PRO A 98130.137 -7.830 18.413 1.00 0.00 N ATOM 1437 CA PRO A 98129.487 -8.797 19.305 1.00 0.00 C ATOM 1438 C PRO A 98128.279 -9.461 18.655 1.00 0.00 C

ATOM 1439 O PRO A 98128.061 -9.336 17.449 1.00 0.00 O ATOM 1440 CB PRO A 98129.050 -7.941 20.495 1.00 0.00 C ATOM 1441 CG PRO A 98128.876 -6.573 19.933 1.00 0.00 C ATOM 1442 CD PRO A 98129.904 -6.437 18.843 1.00 0.00 C ATOM 1443 HA PRO A 98130.179 -9.556 19.637 1.00 0.00 H ATOM 1444 1HB PRO A 98128.126 -8.326 20.898 1.00 0.00 H ATOM 1445 2HB PRO A 98129.817 -7.960 21.256 1.00 0.00 H ATOM 1446 1HG PRO A 98127.881 -6.469 19.526 1.00 0.00 H ATOM 1447 2HG PRO A 98129.046 -5.836 20.703 1.00 0.00 H ATOM 1448 1HD PRO A 98129.515 -5.843 18.029 1.00 0.00 H ATOM 1449 2HD PRO A 98130.810 -5.998 19.233 1.00 0.00 H ATOM 1450 N SER A 99127.494 -10.169 19.462 1.00 0.00 N ATOM 1451 CA SER A 99126.306 -10.854 18.966 1.00 0.00 C ATOM 1452 C SER A 99125.385 -11.247 20.115 1.00 0.00 C ATOM 1453 O SER A 99125.840 -11.743 21.146 1.00 0.00 O ATOM 1454 CB SER A 99126.704 -12.096 18.168 1.00 0.00 C ATOM 1455 OG SER A 99127.637 -11.774 17.150 1.00 0.00 O ATOM 1456 H SER A 99127.719 -10.231 20.413 1.00 0.00 H ATOM 1457 HA SER A 99125.778 -10.172 18.315 1.00 0.00 H ATOM 1458 1HB SER A 99127.153 -12.820 18.832 1.00 0.00 H ATOM 1459 2HB SER A 99125.824 -12.526 17.710 1.00 0.00 H ATOM 1460 HG SER A 99128.438 -12.286 17.275 1.00 0.00 H ATOM 1461 N GLY A 100124.088 -11.024 19.932 1.00 0.00 N ATOM 1462 CA GLY A 100123.124 -11.361 20.963 1.00 0.00 C ATOM 1463 C GLY A 100121.706 -11.447 20.429 1.00 0.00 C ATOM 1464 O GLY A 100120.983 -10.451 20.420 1.00 0.00 O ATOM 1465 H GLY A 100123.782 -10.626 19.090 1.00 0.00 H ATOM 1466 1HA GLY A 100123.394 -12.314 21.393 1.00 0.00 H ATOM 1467 2HA GLY A 100123.161 -10.607 21.736 1.00 0.00 H ATOM 1468 N PRO A 101121.277 -12.635 19.970 1.00 0.00 N ATOM 1469 CA PRO A 101119.927 -12.833 19.431 1.00 0.00 C

ATOM 1470 C PRO A 101118.856 -12.759 20.514 1.00 0.00 C ATOM 1471 O PRO A 101117.797 -12.164 20.313 1.00 0.00 O ATOM 1472 CB PRO A 101119.986 -14.239 18.833 1.00 0.00 C ATOM 1473 CG PRO A 101121.058 -14.933 19.599 1.00 0.00 C ATOM 1474 CD PRO A 101122.072 -13.877 19.941 1.00 0.00 C ATOM 1475 HA PRO A 101119.703 -12.117 18.655 1.00 0.00 H ATOM 1476 1HB PRO A 101119.030 -14.727 18.958 1.00 0.00 H ATOM 1477 2HB PRO A 101120.230 -14.177 17.782 1.00 0.00 H ATOM 1478 1HG PRO A 101120.646 -15.363 20.501 1.00 0.00 H ATOM 1479 2HG PRO A 101121.508 -15.702 18.989 1.00 0.00 H ATOM 1480 1HD PRO A 101122.513 -14.076 20.907 1.00 0.00 H ATOM 1481 2HD PRO A 101122.836 -13.827 19.179 1.00 0.00 H ATOM 1482 N SER A 102119.138 -13.367 21.661 1.00 0.00 N ATOM 1483 CA SER A 102118.198 -13.369 22.776 1.00 0.00 C ATOM 1484 C SER A 102116.891 -14.051 22.386 1.00 0.00 C ATOM 1485 O SER A 102116.548 -14.126 21.206 1.00 0.00 O ATOM 1486 CB SER A 102117.922 -11.938 23.242 1.00 0.00 C ATOM 1487 OG SER A 102118.809 -11.557 24.277 1.00 0.00 O ATOM 1488 H SER A 102119.999 -13.824 21.760 1.00 0.00 H ATOM 1489 HA SER A 102118.650 -13.921 23.588 1.00 0.00 H ATOM 1490 1HB SER A 102118.047 -11.261 22.410 1.00 0.00 H ATOM 1491 2HB SER A 102116.908 -11.872 23.609 1.00 0.00 H ATOM 1492 HG SER A 102119.210 -10.712 24.061 1.00 0.00 H ATOM 1493 N SER A 103116.168 -14.548 23.383 1.00 0.00 N ATOM 1494 CA SER A 103114.898 -15.225 23.144 1.00 0.00 C ATOM 1495 C SER A 103113.728 -14.368 23.617 1.00 0.00 C ATOM 1496 O SER A 103113.660 -13.981 24.784 1.00 0.00 O ATOM 1497 CB SER A 103114.875 -16.578 23.856 1.00 0.00 C ATOM 1498 OG SER A 103115.624 -16.535 25.059 1.00 0.00 O ATOM 1499 H SER A 103116.495 -14.458 24.303 1.00 0.00 H ATOM 1500 HA SER A 103114.804 -15.386 22.081 1.00 0.00 H

ATOM 1501 1HB SER A 103113.855 -16.840 24.093 1.00 0.00 H
ATOM 1502 2HB SER A 103115.299 -17.330 23.208 1.00 0.00 H
ATOM 1503 HG SER A 103116.371 -17.133 24.992 1.00 0.00 H
ATOM 1504 N GLY A 104112.809 -14.076 22.702 1.00 0.00 N
ATOM 1505 CA GLY A 104111.653 -13.267 23.046 1.00 0.00 C
ATOM 1506 C GLY A 104112.037 -11.875 23.512 1.00 0.00 C
ATOM 1507 O GLY A 104111.578 -11.468 24.600 1.00 0.00 O
ATOM 1508 OXT GLY A 104112.796 -11.196 22.791 1.00 0.00 H
ATOM 1510 1HA GLY A 104112.915 -14.411 21.788 1.00 0.00 H
ATOM 1511 2HA GLY A 104111.018 -13.179 22.176 1.00 0.00 H
ATOM 1511 2HA GLY A 104111.103 -13.760 23.833 1.00 0.00 H
ATOM 1512 GLY A 104

Three-Dimensional Structure Coordinate Table 5

ATOM 1 N GLY A 1119.934 2.440 -12.362 1.00 0.00 N ATOM 2 CA GLY A 1120.718 2.882 -11.176 1.00 0.00 C ATOM 3 C GLY A 1121.589 4.087 -11.473 1.00 0.00 C ATOM 4 O GLY A 1122.802 4.050 -11.266 1.00 0.00 O ATOM 5 1H GLY A 1120.404 1.634 -12.822 1.00 0.00 H ATOM 6 2H GLY A 1119.854 3.217 -13.049 1.00 0.00 H ATOM 7 3H GLY A 1118.978 2.151 -12.071 1.00 0.00 H ATOM 8 1HA GLY A 1120.034 3.135 -10.380 1.00 0.00 H ATOM 9 2HA GLY A 1121.348 2.067 -10.851 1.00 0.00 H ATOM10 N SER A 2120.970 5.157 -11.960 1.00 0.00 N ATOM11 CA SER A 2121.698 6.378 -12.287 1.00 0.00 C ATOM12 C SER A 2122.748 6.115 -13.362 1.00 0.00 C ATOM13 O SER A 2123.937 6.005 -13.067 1.00 0.00 O ATOM14 CB SER A 2122.364 6.950 -11.035 1.00 0.00 C ATOM15 OG SER A 2121.480 7.806 -10.331 1.00 0.00 O ATOM16 H SER A 2120.001 5.125 -12.104 1.00 0.00 H

ATOM17 HA SER A 2120.985 7.096 -12.665 1.00 0.00 H ATOM18 1HB SER A 2122.654 6.140 -10.382 1.00 0.00 H ATOM19 2HB SER A 2123.239 7.514 -11.321 1.00 0.00 H ATOM20 HG SER A 2121.576 7.661 -9.387 1.00 0.00 H ATOM21 N SER A 3122.299 6.016 -14.609 1.00 0.00 N ATOM22 CA SER A 3123.200 5.765 -15.728 1.00 0.00 C ATOM23 C SER A 3123.931 4.438 -15.551 1.00 0.00 C ATOM24 O SER A 3123.690 3.708 -14.590 1.00 0.00 O ATOM25 CB SER A 3124.211 6.905 -15.859 1.00 0.00 C ATOM26 OG SER A 3123.566 8.124 -16.188 1.00 0.00 O ATOM27 H SER A 3121.339 6.112 -14.781 1.00 0.00 H ATOM28 HA SER A 3122.605 5.717 -16.628 1.00 0.00 H ATOM29 1HB SER A 3124.734 7.030 -14.923 1.00 0.00 H ATOM30 2HB SER A 3124.919 6.666 -16.639 1.00 0.00 H ATOM31 HG SER A 3122.788 8.233 -15.637 1.00 0.00 H ATOM32 N GLY A 4124.827 4.134 -16.485 1.00 0.00 N ATOM33 CA GLY A 4125.580 2.896 -16.413 1.00 0.00 C ATOM34 C GLY A 4126.815 3.017 -15.541 1.00 0.00 C ATOM35 O GLY A 4127.021 4.037 -14.883 1.00 0.00 O ATOM36 H GLY A 4124.978 4.755 -17.227 1.00 0.00 H ATOM37 1HA GLY A 4124.942 2.122 -16.011 1.00 0.00 H ATOM38 2HA GLY A 4125.883 2.614 -17.411 1.00 0.00 H ATOM39 N SER A 5127.638 1.973 -15.537 1.00 0.00 N ATOM40 CA SER A 5128.859 1.967 -14.740 1.00 0.00 C ATOM41 C SER A 5128.541 2.115 -13.255 1.00 0.00 C ATOM42 O SER A 5127.375 2.182 -12.864 1.00 0.00 O ATOM43 CB SER A 5129.792 3.093 -15.188 1.00 0.00 C ATOM44 OG SER A 5130.310 2.842 -16.482 1.00 0.00 O ATOM45 H SER A 5127.419 1.190 -16.083 1.00 0.00 H ATOM46 HA SER A 5129.352 1.019 -14.897 1.00 0.00 H ATOM47 1HB SER A 5129.245 4.025 -15.208 1.00 0.00 H

ATOM48 2HB SER A 5130.615 3.174 -14.493 1.00 0.00 H ATOM49 HG SER A 5130.634 1.939 -16.528 1.00 0.00 H ATOM50 N SER A 6129.584 2.166 -12.434 1.00 0.00 N ATOM51 CA SER A 6129.415 2.307 -10.992 1.00 0.00 C ATOM52 C SER A 6128.918 3.704 -10.637 1.00 0.00 C ATOM53 O SER A 6128.643 4.519 -11.517 1.00 0.00 O ATOM54 CB SER A 6130.735 2.024 -10.273 1.00 0.00 C ATOM55 OG SER A 6130.834 0.658 -9.907 1.00 0.00 O ATOM56 H SER A 6130.488 2.108 -12.805 1.00 0.00 H ATOM57 HA SER A 6128.680 1.584 -10.673 1.00 0.00 H ATOM58 1HB SER A 6131.558 2.268 -10.928 1.00 0.00 H ATOM59 2HB SER A 6130.794 2.629 -9.380 1.00 0.00 H ATOM60 HG SER A 6131.760 0.409 -9.847 1.00 0.00 H ATOM61 N GLY A 7128.805 3.974 -9.340 1.00 0.00 N ATOM62 CA GLY A 7128.341 5.274 -8.891 1.00 0.00 C ATOM63 C GLY A 7129.005 5.713 -7.601 1.00 0.00 C ATOM64 O GLY A 7129.918 5.051 -7.108 1.00 0.00 O ATOM65 H GLY A 7129.039 3.285 -8.683 1.00 0.00 H ATOM66 1HA GLY A 7128.552 6.003 -9.658 1.00 0.00 H ATOM67 2HA GLY A 7127.273 5.228 -8.736 1.00 0.00 H ATOM68 N LEUA 8128.544 6.833 -7.053 1.00 0.00 N ATOM69 CA LEU A 8129.099 7.360 -5.811 1.00 0.00 C ATOM70 C LEUA 8127.992 7.667 -4.808 1.00 0.00 C ATOM71 O LEUA 8126.829 7.822 -5.180 1.00 0.00 O ATOM72 CB LEU A 8129,916 8.624 -6.089 1.00 0.00 C ATOM73 CG LEU A 8131.353 8.378 -6.550 1.00 0.00 C ATOM74 CD1 LEU A 8131.955 9.650 -7.124 1.00 0.00 C ATOM75 CD2 LEU A 8132.199 7.859 -5.397 1.00 0.00 C ATOM76 H LEUA 8127.814 7.315 -7.493 1.00 0.00 H ATOM77 HA LEU A 8129.750 6.607 -5.392 1.00 0.00 H ATOM78 1HB LEU A 8129.407 9.194 -6.854 1.00 0.00 H

ATOM79 2HB LEU A 8129.947 9.213 -5.186 1.00 0.00 H ATOM80 HG LEU A 8131.352 7.628 -7.328 1.00 0.00 H ATOM81 1HD1 LEU A 8131.820 10.461 -6.423 1.00 0.00 H ATOM82 2HD1 LEU A 8131.462 9.894 -8.054 1.00 0.00 H ATOM83 3HD1 LEU A 8133.010 9.501 -7.304 1.00 0.00 H ATOM84 1HD2 LEU A 8132.928 7.157 -5.772 1.00 0.00 H ATOM85 2HD2 LEU A 8131.562 7.367 -4.676 1.00 0.00 H ATOM86 3HD2 LEU A 8132,706 8.686 -4.922 1.00 0.00 H ATOM87 N ALAA 9128.361 7.754 -3.534 1.00 0.00 N ATOM88 CA ALA A 9127.398 8.042 -2.478 1.00 0.00 C ATOM89 C ALAA 9128.053 8.796 -1.326 1.00 0.00 C ATOM90 O ALAA 9127.633 8.677 -0.176 1.00 0.00 O ATOM91 CB ALA A 9126.766 6.754 -1.975 1.00 0.00 C ATOM92 H ALAA 9129.303 7.619 -3.299 1.00 0.00 H ATOM93 HA ALA A 9126.617 8.658 -2.899 1.00 0.00 H ATOM94 1HB ALA A 9127.284 6.421 -1.087 1.00 0.00 H ATOM95 2HB ALA A 9126.839 5.994 -2.740 1.00 0.00 H ATOM96 3HB ALA A 9125.726 6.929 -1.742 1.00 0.00 H ATOM97 N MET A 10129.085 9.573 -1.643 1.00 0.00 N ATOM98 CA MET A 10129.796 10.347 -0.633 1.00 0.00 C ATOM99 C MET A 10130.666 11.422 -1.282 1.00 0.00 C ATOM 100 O MET A 10131.871 11.241 -1.449 1.00 0.00 O 101 CB META 10130.664 9.427 0.230 1.00 0.00 C ATOM ATOM 102 CG MET A 10130.012 9.038 1.548 1.00 0.00 C 103 SD META 10130.760 9.864 2.965 1.00 0.00 S ATOM **ATOM** 104 CE META 10132.424 9.208 2.903 1.00 0.00 C 105 H META 10129.373 9.628 -2.578 1.00 0.00 H ATOM 106 HA META 10129.061 10.827 -0.005 1.00 0.00 H ATOM 107 1HB MET A 10130.870 8.525 -0.325 1.00 0.00 H ATOM 108 2HB MET A 10131.596 9.928 0.446 1.00 0.00 H ATOM ATOM 109 1HG MET A 10128.966 9.301 1.508 1.00 0.00 H

110 2HG MET A 10130.109 7.970 1.680 1.00 0.00 H 111 1HE MET A 10132.73,2 9.103 1.872 1.00 0.00 H **ATOM ATOM** 112 2HE MET A 10132.449 8.242 3.384 1.00 0.00 H 113 3HE MET A 10133.098 9.881 3.412 1.00 0.00 H ATOM 114 N PRO A 11130.060 12.563 -1.655 1.00 0.00 N ATOM ATOM 115 CA PRO A 11130.787 13.668 -2.285 1.00 0.00 C 116 C PROA 11131.997 14.110 -1.464 1.00 0.00 C **ATOM** 117 O PRO A 11133.081 14.317 -2.011 1.00 0.00 O ATOM 118 CB PRO A 11129.751 14.793 -2.359 1.00 0.00 C ATOM 119 CG PRO A 11128.428 14.110 -2.301 1.00 0.00 C ATOM ATOM 120 CD PRO A 11128.627 12.861 -1.489 1.00 0.00 C **ATOM** 121 HA PRO A 11131.110 13.409 -3.282 1.00 0.00 H 122 1HB PRO A 11129.886 15.465 -1.524 1.00 0.00 H ATOM 123 2HB PRO A 11129.873 15.335 -3.285 1.00 0.00 H ATOM ATOM 124 1HG PRO A 11127.708 14.752 -1.821 1.00 0.00 H ATOM 125 2HG PRO A 11128.101 13.859 -3.300 1.00 0.00 H ATOM 126 1HD PRO A 11128.392 13.045 -0.451 1.00 0.00 H 127 2HD PRO A 11128.020 12.057 -1.877 1.00 0.00 H ATOM **ATOM** 128 N PRO A 12131.836 14.258 -0.134 1.00 0.00 N 129 CA PRO A 12132.932 14.672 0.747 1.00 0.00 C ATOM 130 C PRO A 12134.071 13.659 0.754 1.00 0.00 C ATOM ATOM 131 O PROA 12135.204 13.984 1.107 1.00 0.00 O 132 CB PRO A 12132.283 14.754 2.136 1.00 0.00 C ATOM 133 CG PRO A 12130.815 14.809 1.879 1.00 0.00 C ATOM 134 CD PRO A 12130.591 14.030 0.616 1.00 0.00 C ATOM 135 HA PRO A 12133.318 15.642 0.469 1.00 0.00 H ATOM ATOM 136 1HB PRO A 12132.549 13.879 2.711 1.00 0.00 H 137 2HB PRO A 12132.626 15.641 2.644 1.00 0.00 H ATOM ATOM 138 1HG PRO A 12130.281 14.354 2.700 1.00 0.00 H ATOM 139 2HG PRO A 12130.502 15.834 1.748 1.00 0.00 H ATOM 140 1HD PRO A 12130.458 12.981 0.837 1.00 0.00 H

141 2HD PRO A 12129.738 14.416 0.081 1.00 0.00 H **ATOM** 142 N GLYA 13133.759 12.427 0.361 1.00 0.00 N 143 CA GLY A 13134.766 11.384 0.327 1.00 0.00 C ATOM 144 C GLY A 13135.229 11.068 -1.082 1.00 0.00 C **ATOM** 145 O GLY A 13134.684 11.593 -2.053 1.00 0.00 O ATOM ATOM 146 H GLY A 13132.837 12.226 0.090 1.00 0.00 H ATOM 147 1HA GLY A 13135.617 11.700 0.911 1.00 0.00 H **ATOM** 148 2HA GLY A 13134.355 10.487 0.768 1.00 0.00 H **ATOM** 149 N ASNA 14136.236 10.209 -1.194 1.00 0.00 N **ATOM** 150 CA ASN A 14136.770 9.824 -2.495 1.00 0.00 C ATOM 151 C ASN A 14135.847 8.829 -3.190 1.00 0.00 C **ATOM** 152 O ASN A 14135.407 9.058 -4.316 1.00 0.00 O **ATOM** 153 CB ASN A 14138.167 9.219 -2.337 1.00 0.00 C **ATOM** 154 CG ASN A 14139.066 10.061 -1.454 1.00 0.00 C **ATOM** 155 OD1 ASN A 14139.732 10.984 -1.925 1.00 0.00 O ATOM 156 ND2 ASN A 14139.090 9.749 -0.164 1.00 0.00 N **ATOM** 157 H ASN A 14136.629 9.823 -0.383 1.00 0.00 H ATOM 158 HA ASN A 14136.841 10.715 -3.100 1.00 0.00 H ATOM 159 1HB ASN A 14138.079 8.237 -1.896 1.00 0.00 H **ATOM** 160 2HB ASN A 14138.627 9.133 -3.310 1.00 0.00 H 161 1HD2 ASN A 14138.535 9.002 0.142 1.00 0.00 H ATOM **ATOM** 162 2HD2 ASN A 14139.663 10.277 0.430 1.00 0.00 H ATOM 163 N SER A 15135.560 7.722 -2.512 1.00 0.00 N 164 CA SER A 15134.689 6.693 -3.065 1.00 0.00 C ATOM **ATOM** 165 C SER A 15133.686 6.210 -2.022 1.00 0.00 C 166 O SER A 15132.492 6.099 -2.300 1.00 0.00 O **ATOM** ATOM 167 CB SER A 15135.520 5.512 -3.574 1.00 0.00 C **ATOM** 168 OG SER A 15134.733 4:638 -4.365 1.00 0.00 O 169 H SER A 15135.942 7.596 -1.618 1.00 0.00 H ATOM

ATOM

ATOM

170 HA SER A 15134.149 7.125 -3.893 1.00 0.00 H

171 1HB SER A 15136.337 5.884 -4.175 1.00 0.00 H

172 2HB SER A 15135.913 4.962 -2.732 1.00 0.00 H ATOM 173 HG SER A 15133.932 4.410 -3.889 1.00 0.00 H ATOM 174 N HIS A 16134.179 5.924 -0.822 1.00 0.00 N ATOM **ATOM** 175 CA HIS A 16133.325 5.452 0.263 1.00 0.00 C 176 C HIS A 16133.925 5.807 1.620 1.00 0.00 C ATOM 177 O HIS A 16133.233 6.314 2.502 1.00 0.00 O ATOM ATOM 178 CB HIS A 16133.124 3.940 0.160 1.00 0.00 C 179 CG HIS A 16131.734 3.497 0.497 1.00 0.00 C ATOM **ATOM** 180 ND1 HIS A 16131.293 3.324 1.793 1.00 0.00 N 181 CD2 HIS A 16130.683 3.192 -0.300 1.00 0.00 C **ATOM** 182 CE1 HIS A 16130.032 2.931 1.777 1.00 0.00 C ATOM **ATOM** 183 NE2 HIS A 16129.638 2.843 0.520 1.00 0.00 N 184 H HIS A 16135.140 6.032 -0.662 1.00 0.00 H **ATOM** ATOM 185 HA HIS A 16132.367 5.942 0.166 1.00 0.00 H **ATOM** 186 1HB HIS A 16133.337 3.623 -0.849 1.00 0.00 H ATOM 187 2HB HIS A 16133.806 3.445 0.838 1.00 0.00 H **ATOM** 188 HD1 HIS A 16131.825 3.467 2.603 1.00 0.00 H 189 HD2 HIS A 16130.670 3.217 -1.381 1.00 0.00 H **ATOM** 190 HE1 HIS A 16129.425 2.718 2.646 1.00 0.00 H **ATOM ATOM** 191 HE2 HIS A 16128.774 2.491 0.222 1.00 0.00 H 192 N GLY A 17135.217 5.537 1.779 1.00 0.00 N **ATOM** ATOM 193 CA GLYA 17135.887 5.834 3.032 1.00 0.00 C 194 C GLY A 17137.270 5.217 3.109 1.00 0.00 C ATOM 195 O GLY A 17137.577 4.481 4.045 1.00 0.00 O **ATOM ATOM** 196 H GLY A 17135.718 5.132 1.041 1.00 0.00 H 197 1HA GLY A 17135.976 6.905 3.134 1.00 0.00 H ATOM ATOM 198 2HA GLY A 17135.289 5.453 3.846 1.00 0.00 H ATOM 199 N LEUA 18138.106 5.519 2.121 1.00 0.00 N 200 CA LEU A 18139.464 4.989 2.080 1.00 0.00 C ATOM 201 C LEUA 18140.482 6.077 2.411 1.00 0.00 C **ATOM** ATOM 202 O LEUA 18140.788 6.929 1.578 1.00 0.00 O

203 CB LEU A 18139.763 4.398 0.701 1.00 0.00 C **ATOM** 204 CG LEUA 18139.023 3.098 0.381 1.00 0.00 C ATOM ATOM 205 CD1 LEU A 18138.916 2.902 -1.124 1.00 0.00 C 206 CD2 LEU A 18139.726 1.914 1.027 1.00 0.00 C ATOM 207 H LEU A 18137.802 6.112 1.403 1.00 0.00 H ATOM 208 HA LEUA 18139.537 4.207 2.821 1.00 0.00 H ATOM ATOM 209 1HB LEU A 18139.500 5.133 -0.046 1.00 0.00 H 210 2HB LEU A 18140.824 4.207 0.636 1.00 0.00 H **ATOM ATOM** 211 HG LEUA 18138.021 3.154 0.781 1.00 0.00 H 212 1HD1 LEU A 18138.964 1.848 -1.354 1.00 0.00 H ATOM 213 2HD1 LEU A 18139.732 3.415 -1.612 1.00 0.00 H ATOM **ATOM** 214 3HD1 LEU A 18137.978 3.305 -1.473 1.00 0.00 H 215 1HD2 LEU A 18139.773 2.062 2.095 1.00 0.00 H ATOM 216 2HD2 LEU A 18140.726 1.828 0.630 1.00 0.00 H ATOM 217 3HD2 LEU A 18139.175 1.009 0.813 1.00 0.00 H ATOM 218 N GLUA 19141.003 6.039 3.633 1.00 0.00 N ATOM 219 CA GLUA 19141.987 7.021 4.076 1.00 0.00 C **ATOM** 220 C GLUA 19143.003 6.385 5.019 1.00 0.00 C ATOM 221 O GLUA 19142.915 5.198 5.333 1.00 0.00 O ATOM 222 CB GLU A 19141.291 8.193 4.771 1.00 0.00 C ATOM 223 CG GLU A 19140.354 7.767 5.889 1.00 0.00 C **ATOM** 224 CD GLUA 19139.186 8.717 6.064 1.00 0.00 C **ATOM** ATOM 225 OE1 GLU A 19138.168 8.543 5.361 1.00 0.00 O 226 OE2 GLU A 19139.287 9.634 6.905 1.00 0.00 O ATOM 227 H GLUA 19140.719 5.335 4.253 1.00 0.00 H ATOM 228 HA GLU A 19142.504 7.388 3.202 1.00 0.00 H **ATOM** 229 1HB GLU A 19142.043 8.845 5.190 1.00 0.00 H ATOM 230 2HB GLU A 19140.717 8.741 4.040 1.00 0.00 H **ATOM** 231 1HG GLU A 19139.968 6.784 5.664 1.00 0.00 H ATOM 232 2HG GLU A 19140.911 7.730 6.814 1.00 0.00 H ATOM ATOM 233 N VALA 20143.968 7.183 5.466 1.00 0.00 N

234 CA VALA 20145.001 6.699 6.374 1.00 0.00 C ATOM 235 C VALA 20144.390 6.120 7.646 1.00 0.00 C 236 O VALA 20143.480 6.706 8.230 1.00 0.00 O **ATOM ATOM** 237 CB VALA 20145.985 7.822 6.754 1.00 0.00 C **ATOM** 238 CG1 VAL A 20147.147 7.267 7.563 1.00 0.00 C 239 CG2 VAL A 20146.487 8.537 5.508 1.00 0.00 C **ATOM** 240 H VALA 20143.984 8.120 5.180 1.00 0.00 H ATOM 241 HA VALA 20145.554 5.922 5.865 1.00 0.00 H **ATOM** 242 HB VALA 20145.460 8.540 7.368 1.00 0.00 H 243 1HG1 VAL A 20147.999 7.923 7.468 1.00 0.00 H **ATOM** 244 2HG1 VAL A 20147.406 6.286 7.194 1.00 0.00 H **ATOM** 245 3HG1 VAL A 20146.861 7.195 8.602 1.00 0.00 H ATOM **ATOM** 246 1HG2 VAL A 20146.440 7.864 4.665 1.00 0.00 H 247 2HG2 VAL A 20147.508 8.853 5.661 1.00 0.00 H ATOM 248 3HG2 VAL A 20145.868 9.401 5.315 1.00 0.00 H ATOM 249 N GLY A 21144.897 4.967 8.068 1.00 0.00 N ATOM 250 CA GLY A 21144.389 4.329 9.267 1.00 0.00 C **ATOM** ATOM 251 C GLY A 21143.329 3.289 8.967 1.00 0.00 C ATOM 252 O GLY A 21143.299 2.225 9.586 1.00 0.00 O 253 H GLY A 21145.624 4.546 7.561 1.00 0.00 H ATOM 254 1HA GLY A 21145.208 3.852 9.784 1.00 0.00 H **ATOM** 255 2HA GLY A 21143.963 5.084 9.912 1.00 0.00 H ATOM 256 N SER A 22142.455 3.595 8.013 1.00 0.00 N **ATOM ATOM** 257 CA SER A 22141.387 2.679 7.631 1.00 0.00 C 258 C SER A 22141.933 1.524 6.796 1.00 0.00 C ATOM 259 O SER A 22142.942 1.668 6.106 1.00 0.00 O **ATOM** 260 CB SER A 22140.304 3.423 6.847 1.00 0.00 C **ATOM** 261 OG SER A 22140.042 4.693 7.418 1.00 0.00 O **ATOM ATOM** 262 H SER A 22142.530 4.459 7.555 1.00 0.00 H 263 HA SER A 22140.953 2.280 8.535 1.00 0.00 H **ATOM** ATOM 264 1HB SER A 22140.632 3.561 5.828 1.00 0.00 H

265 2HB SER A 22139.393 2.842 6.856 1.00 0.00 H 266 HG SER A 22139.251 5.065 7.021 1.00 0.00 H **ATOM** 267 N LEUA 23141.259 0.381 6.865 1.00 0.00 N ATOM 268 CA LEU A 23141.677 -0.798 6.116 1.00 0.00 C **ATOM** 269 C LEUA 23141.131 -0.761 4.693 1.00 0.00 C ATOM 270 O LEUA 23140.073 -0.186 4.438 1.00 0.00 O ATOM ATOM 271 CB LEU A 23141.206 -2.070 6.824 1.00 0.00 C 272 CG LEU A 23141.688 -2.224 8.267 1.00 0.00 C ATOM 273 CD1 LEU A 23140.698 -3.049 9.075 1.00 0.00 C ATOM 274 CD2 LEU A 23143.069 -2.862 8.302 1.00 0.00 C ATOM 275 H LEUA 23140.463 0.329 7.434 1.00 0.00 H **ATOM** ATOM 276 HA LEU A 23142.756 -0.799 6.074 1.00 0.00 H 277 1HB LEU A 23140.126 -2.077 6.823 1.00 0.00 H **ATOM** 278 2HB LEU A 23141.555 -2.921 6.259 1.00 0.00 H ATOM 279 HG LEU A 23141.758 -1.248 8.722 1.00 0.00 H ATOM 280 1HD1 LEU A 23140.860 -4.098 8.880 1.00 0.00 H ATOM **ATOM** 281 2HD1 LEU A 23139.691 -2.781 8.791 1.00 0.00 H 282 3HD1 LEU A 23140.840 -2.852 10.127 1.00 0.00 H **ATOM** 283 1HD2 LEU A 23143.649 -2.423 9.100 1.00 0.00 H ATOM 284 2HD2 LEU A 23143.568 -2.691 7.359 1.00 0.00 H **ATOM** 285 3HD2 LEU A 23142.970 -3.924 8.469 1.00 0.00 H ATOM **ATOM** 286 N ALAA 24141.859 -1.379 3.768 1.00 0.00 N 287 CA ALAA 24141.447 -1.417 2.370 1.00 0.00 C ATOM 288 C ALAA 24141.974 -2.668 1.676 1.00 0.00 C ATOM 289 O ALAA 24142.870 -3.341 2.186 1.00 0.00 O **ATOM** 290 CB ALA A 24141.925 -0.168 1.646 1.00 0.00 C **ATOM** 291 H ALAA 24142.693 -1.820 4.032 1.00 0.00 H **ATOM ATOM** 292 HA ALAA 24140.367 -1.430 2.341 1.00 0.00 H 293 1HB ALAA 24141.383 -0.061 0.718 1.00 0.00 H **ATOM** 294 2HB ALAA 24142.981 -0.255 1.439 1.00 0.00 H **ATOM** 295 3HB ALAA 24141.749 0.698 2.267 1.00 0.00 H ATOM

296 N GLUA 25141.413 -2.975 0.511 1.00 0.00 N ATOM **ATOM** 297 CA GLU A 25141.827 -4.145 -0.252 1.00 0.00 C **ATOM** 298 C GLU A 25142.061 -3.785 -1.716 1.00 0.00 C 299 O GLUA 25141.346 -2.961 -2.285 1.00 0.00 O **ATOM** 300 CB GLU A 25140.773 -5.248 -0.147 1.00 0.00 C **ATOM ATOM** 301 CG GLU A 25141.270 -6.611 -0.600 1.00 0.00 C **ATOM** 302 CD GLU A 25140.237 -7.371 -1.407 1.00 0.00 C 303 OE1 GLU A 25139.590 -8.277 -0.841 1.00 0.00 O ATOM **ATOM** 304 OE2 GLU A 25140.072 -7.060 -2.605 1.00 0.00 O 305 H GLU A 25140.703 -2.399 0.156 1.00 0.00 H **ATOM** 306 HA GLUA 25142.754 -4.505 0.169 1.00 0.00 H **ATOM ATOM** 307 1HB GLU A 25140.453 -5.328 0.880 1.00 0.00 H 308 2HB GLU A 25139.924 -4.978 -0.760 1.00 0.00 H **ATOM** 309 1HG GLU A 25142.151 -6.474 -1.210 1.00 0.00 H **ATOM** 310 2HG GLU A 25141.525 -7.194 0.273 1.00 0.00 H **ATOM** 311 N VALA 26143.066 -4.410 -2.321 1.00 0.00 N ATOM 312 CA VAL A 26143.394 -4.156 -3.718 1.00 0.00 C **ATOM** 313 C VALA 26142.998 -5.336 -4.599 1.00 0.00 C ATOM 314 O VALA 26143.026 -6.486 -4.161 1.00 0.00 O ATOM **ATOM** 315 CB VAL A 26144.898 -3.876 -3.901 1.00 0.00 C 316 CG1 VAL A 26145.188 -3.419 -5.322 1.00 0.00 C **ATOM** 317 CG2 VAL A 26145.374 -2.841 -2.892 1.00 0.00 C **ATOM ATOM** 318 H VALA 26143.601 -5.057 -1.815 1.00 0.00 H 319 HA VALA 26142.845 -3.282 -4.036 1.00 0.00 H **ATOM** 320 HB VALA 26145.438 -4.794 -3.724 1.00 0.00 H **ATOM** 321 1HG1 VAL A 26144.303 -2.967 -5.743 1.00 0.00 H **ATOM** 322 2HG1 VAL A 26145.477 -4.270 -5.921 1.00 0.00 H **ATOM ATOM** 323 3HG1 VAL A 26145.990 -2.697 -5.311 1.00 0.00 H 324 1HG2 VAL A 26145.426 -3.291 -1.912 1.00 0.00 H ATOM 325 2HG2 VAL A 26144.682 -2.013 -2.872 1.00 0.00 H **ATOM** 326 3HG2 VAL A 26146.354 -2.485 -3.177 1.00 0.00 H

ATOM

327 N LYS A 27142.631 -5.043 -5.842 1.00 0.00 N **ATOM** 328 CA LYS A 27142.230 -6.080 -6.785 1.00 0.00 C ATOM 329 C LYS A 27143.429 -6.587 -7.579 1.00 0.00 C ATOM 330 O LYS A 27143.642 -6.187 -8.723 1.00 0.00 O ATOM 331 CB LYS A 27141.161 -5.544 -7.739 1.00 0.00 C **ATOM** 332 CG LYS A 27139.740 -5.743 -7.235 1.00 0.00 C ATOM **ATOM** 333 CD LYS A 27139.084 -6.954 -7.879 1.00 0.00 C **ATOM** 334 CE LYS A 27139.179 -8.181 -6.985 1.00 0.00 C 335 NZ LYS A 27139.457 -9.418 -7.765 1.00 0.00 N **ATOM** 336 H LYS A 27142.630 -4.106 -6.132 1.00 0.00 H ATOM 337 HA LYS A 27141.815 -6.900 -6.219 1.00 0.00 H **ATOM** ATOM 338 1HB LYS A 27141.323 -4.487 -7.886 1.00 0.00 H 339 2HB LYS A 27141.257 -6.049 -8.689 1.00 0.00 H ATOM 340 1HG LYS A 27139.765 -5.886 -6.166 1.00 0.00 H ATOM 341 2HG LYS A 27139.159 -4.863 -7.470 1.00 0.00 H **ATOM** ATOM 342 1HD LYS A 27138.044 -6.734 -8.061 1.00 0.00 H ATOM 343 2HD LYS A 27139.579 -7.164 -8.816 1.00 0.00 H 344 1HE LYS A 27139.976 -8.030 -6.272 1.00 0.00 H **ATOM** 345 2HE LYS A 27138.244 -8.299 -6.459 1.00 0.00 H ATOM **ATOM** 346 1HZ LYS A 27138.945 -10.223 -7.353 1.00 0.00 H 347 2HZ LYS A 27140.475 -9.627 -7.756 1.00 0.00 H ATOM **ATOM** 348 3HZ LYS A 27139.150 -9.294 -8.752 1.00 0.00 H 349 N GLU A 28144.209 -7.469 -6.964 1.00 0.00 N ATOM 350 CA GLUA 28145.388 -8.032 -7.613 1.00 0.00 C ATOM 351 C GLUA 28145.339 -9.556 -7.602 1.00 0.00 C ATOM 352 O GLUA 28144.374 -10.153 -7.126 1.00 0.00 O ATOM 353 CB GLU A 28146.661 -7.544 -6.918 1.00 0.00 C ATOM 354 CG GLU A 28147.726 -7.045 -7.879 1.00 0.00 C ATOM 355 CD GLU A 28148.621 -5.987 -7.262 1.00 0.00 C **ATOM** 356 OE1 GLU A 28148.123 -4.875 -6.987 1.00 0.00 O ATOM 357 OE2 GLU A 28149.819 -6.271 -7.052 1.00 0.00 O ATOM

358 H GLUA 28143.987 -7.749 -6.051 1.00 0.00 H **ATOM** 359 HA GLUA 28145.396 -7.691 -8.638 1.00 0.00 H ATOM 360 1HB GLU A 28146.405 -6.736 -6.249 1.00 0.00 H ATOM 361 2HB GLUA 28147.079 -8.356 -6.341 1.00 0.00 H ATOM 362 1HG GLUA 28148.340 -7.880 -8.183 1.00 0.00 H ATOM 363 2HG GLU A 28147.241 -6.623 -8.748 1.00 0.00 H ATOM 364 N ASNA 29146.388 -10.180 -8.131 1.00 0.00 N ATOM 365 CA ASN A 29146.464 -11.635 -8.182 1.00 0.00 C **ATOM** 366 C ASN A 29146.473 -12.229 -6.774 1.00 0.00 C **ATOM** 367 O ASN A 29145.597 -13.017 -6.419 1.00 0.00 O ATOM **ATOM** 368 CB ASN A 29147.717 -12.075 -8.943 1.00 0.00 C 369 CG ASN A 29147.423 -12.410 -10.393 1.00 0.00 C ATOM 370 OD1 ASN A 29147.664 -13.530 -10.844 1.00 0.00 O **ATOM** 371 ND2 ASN A 29146.902 -11.437 -11.130 1.00 0.00 N **ATOM** 372 H ASN A 29147.126 -9.650 -8.495 1.00 0.00 H ATOM ATOM 373 HA ASN A 29145.590 -11.995 -8.705 1.00 0.00 H 374 1HB ASN A 29148.444 -11.278 -8.918 1.00 0.00 H ATOM 375 2HB ASN A 29148.132 -12.951 -8.467 1.00 0.00 H **ATOM** 376 1HD2 ASN A 29146.737 -10.570 -10.704 1.00 0.00 H **ATOM** 377 2HD2 ASN A 29146.701 -11.625 -12.071 1.00 0.00 H **ATOM** 378 N PRO A 30147.468 -11.853 -5.951 1.00 0.00 N ATOM **ATOM** 379 CA PRO A 30147.587 -12.350 -4.578 1.00 0.00 C 380 C PRO A 30146.604 -11.669 -3.628 1.00 0.00 C ATOM 381 O PROA 30146.755 -10.489 -3.310 1.00 0.00 O **ATOM** 382 CB PRO A 30149.025 -11.990 -4.206 1.00 0.00 C ATOM 383 CG PRO A 30149.325 -10.773 -5.008 1.00 0.00 C ATOM 384 CD PRO A 30148.555 -10.915 -6.295 1.00 0.00 C **ATOM** 385 HA PRO A 30147.456 -13.420 -4.531 1.00 0.00 H ATOM 386 1HB PRO A 30149.086 -11.793 -3.146 1.00 0.00 H ATOM 387 2HB PRO A 30149.682 -12.806 -4.465 1.00 0.00 H ATOM ATOM 388 1HG PRO A 30149.001 -9.892 -4.474 1.00 0.00 H

389 2HG PRO A 30150.385 -10.720 -5.212 1.00 0.00 H **ATOM** 390 1HD PRO A 30148.156 -9.960 -6.602 1.00 0.00 H **ATOM** 391 2HD PRO A 30149.186 -11.325 -7.069 1.00 0.00 H ATOM 392 N PRO A 31145.579 -12.403 -3.156 1.00 0.00 N **ATOM** 393 CA PRO A 31144.575 -11.854 -2.239 1.00 0.00 C **ATOM** 394 C PRO A 31145.149 -11.573 -0.854 1.00 0.00 C ATOM ATOM 395 O PRO A 31145.083 -12.418 0.038 1.00 0.00 O 396 CB PRO A 31143.517 -12.957 -2.165 1.00 0.00 C **ATOM** 397 CG PRO A 31144.253 -14.209 -2.491 1.00 0.00 C **ATOM** 398 CD PRO A 31145.317 -13.819 -3.478 1.00 0.00 C ATOM 399 HA PRO A 31144.132 -10.951 -2.633 1.00 0.00 H **ATOM** ATOM 400 1HB PRO A 31143.097 -12.991 -1.170 1.00 0.00 H 401 2HB PRO A 31142.737 -12.761 -2.885 1.00 0.00 H **ATOM** 402 1HG PRO A 31144.703 -14.614 -1.596 1.00 0.00 H ATOM 403 2HG PRO A 31143.580 -14.929 -2.931 1.00 0.00 H ATOM 404 1HD PRO A 31146.205 -14.418 -3.334 1.00 0.00 H ATOM **ATOM** 405 2HD PRO A 31144.950 -13.923 -4.488 1.00 0.00 H 406 N PHE A 32145.712 -10.382 -0.683 1.00 0.00 N ATOM: 407 CA PHE A 32146.298 -9.990 0.593 1.00 0.00 C ATOM ATOM 408 C PHE A 32145.431 -8.947 1.292 1.00 0.00 C 409 O PHE A 32144.494 -8.408 0.703 1.00 0.00 O ATOM **ATOM** 410 CB PHEA 32147.709 -9.437 0.382 1.00 0.00 C **ATOM** 411 CG PHE A 32147.801 -8.437 -0.735 1.00 0.00 C 412 CD1 PHE A 32148.541 -8.716 -1.873 1.00 0.00 C **ATOM** 413 CD2 PHE A 32147.149 -7.218 -0.646 1.00 0.00 C ATOM 414 CE1 PHE A 32148.628 -7.799 -2.902 1.00 0.00 C **ATOM** 415 CE2 PHE A 32147.233 -6.295 -1.672 1.00 0.00 C ATOM 416 CZ PHE A 32147.973 -6.586 -2.801 1.00 0.00 C **ATOM** 417 H PHE A 32145.734 -9.751 -1.433 1.00 0.00 H ATOM 418 HA PHE A 32146.355 -10.870 1.216 1.00 0.00 H ATOM ATOM 419 1HB PHE A 32148.038 -8.952 1.289 1.00 0.00 H

ATOM 420 2HB PHE A 32148.377 -10.254 0.155 1.00 0.00 H 421 HD1 PHE A 32149.052 -9.664 -1.952 1.00 0.00 H ATOM 422 HD2 PHE A 32146.571 -6.989 0.237 1.00 0.00 H **ATOM** 423 HE1 PHE A 32149.208 -8.027 -3.784 1.00 0.00 H ATOM ATOM 424 HE2 PHE A 32146.719 -5.348 -1.590 1.00 0.00 H ATOM 425 HZ PHE A 32148.039 -5.867 -3.604 1.00 0.00 H 426 N TYR A 33145.750 -8.668 2.552 1.00 0.00 N **ATOM** 427 CA TYR A 33145.000 -7.690 3.332 1.00 0.00 C ATOM 428 C TYR A 33145.940 -6.694 4.004 1.00 0.00 C ATOM 429 O TYR A 33146.852 -7.081 4.734 1.00 0.00 O ATOM 430 CB TYR A 33144.147 -8.395 4.388 1.00 0.00 C ATOM 431 CG TYR A 33142.780 -8.803 3.888 1.00 0.00 C ATOM 432 CD1 TYR A 33141.996 -7.922 3.154 1.00 0.00 C **ATOM** 433 CD2 TYR A 33142.273 -10.070 4.151 1.00 0.00 C **ATOM** 434 CE1 TYR A 33140.746 -8.291 2.696 1.00 0.00 C ATOM ATOM 435 CE2 TYR A 33141.023 -10.447 3.696 1.00 0.00 C 436 CZ TYR A 33140.264 -9.554 2.970 1.00 0.00 C ATOM 437 OH TYR A 33139.019 -9.926 2.514 1.00 0.00 O **ATOM** 438 H TYR A 33146.508 -9.131 2.967 1.00 0.00 H **ATOM** 439 HA TYR A 33144.351 -7.155 2.655 1.00 0.00 H **ATOM** ATOM 440 1HB TYR A 33144.659 -9.288 4.717 1.00 0.00 H 441 2HB TYR A 33144.010 -7.734 5.230 1.00 0.00 H ATOM 442 HD1 TYR A 33142.376 -6.934 2.941 1.00 0.00 H ATOM 443 HD2 TYR A 33142.869 -10.766 4.721 1.00 0.00 H **ATOM** 444 HE1 TYR A 33140.152 -7.592 2.126 1.00 0.00 H **ATOM** 445 HE2 TYR A 33140.646 -11.436 3.910 1.00 0.00 H **ATOM** 446 HH TYR A 33139.088 -10.756 2.037 1.00 0.00 H ATOM 447 N GLY A 34145.710 -5.410 3.751 1.00 0.00 N ATOM 448 CA GLY A 34146.544 -4.378 4.337 1.00 0.00 C **ATOM** 449 C GLY A 34145.757 -3.138 4.711 1.00 0.00 C ATOM ATOM 450 O GLY A 34144.578 -3.019 4.378 1.00 0.00 O

451 H GLY A 34144.969 -5.161 3.160 1.00 0.00 H **ATOM** 452 1HA GLY A 34147.016 -4.774 5.225 1.00 0.00 H 453 2HA GLY A 34147.312 -4.103 3.628 1.00 0.00 H **ATOM** ATOM 454 N VALA 35146.409 -2.212 5.406 1.00 0.00 N ATOM 455 CA VALA 35145.764 -0.974 5.827 1.00 0.00 C **ATOM** 456 C VALA 35146.453 0.240 5.212 1.00 0.00 C 457 O VALA 35147.668 0.241 5.013 1.00 0.00 O ATOM **ATOM** 458 CB VALA 35145.763 -0.835 7.362 1.00 0.00 C **ATOM** 459 CG1 VALA 35147.187 -0.811 7.901 1.00 0.00 C 460 CG2 VAL A 35145.001 0.411 7.788 1.00 0.00 C ATOM 461 H VALA 35147.348 -2.365 5.642 1.00 0.00 H **ATOM** 462 HA VALA 35144.738 -1.002 5.489 1.00 0.00 H ATOM **ATOM** 463 HB VALA 35145.262 -1.697 7.781 1.00 0.00 H 464 1HG1 VAL A 35147.865 -0.519 7.113 1.00 0.00 H ATOM **ATOM** 465 2HG1 VAL A 35147.453 -1.795 8.258 1.00 0.00 H 466 3HG1 VAL A 35147.252 -0.103 8.714 1.00 0.00 H ATOM 467 1HG2 VAL A 35145.141 0.574 8.847 1.00 0.00 H ATOM **ATOM** 468 2HG2 VAL A 35143.950 0.278 7.581 1.00 0.00 H 469 3HG2 VAL A 35145.372 1.265 7.241 1.00 0.00 H ATOM 470 N ILE A 36145.670 1.271 4.913 1.00 0.00 N ATOM 471 CA ILE A 36146.207 2.491 4.322 1.00 0.00 C **ATOM** 472 C ILE A 36147.127 3.214 5.300 1.00 0.00 C ATOM 473 O ILE A 36146.803 3.363 6.478 1.00 0.00 O **ATOM** ATOM 474 CB ILE A 36145.080 3.449 3.888 1.00 0.00 C 475 CG1 ILE A 36144.064 2.715 3.011 1.00 0.00 C ATOM 476 CG2 ILE A 36145.658 4.648 3.147 1.00 0.00 C ATOM 477 CD1 ILE A 36142.904 3.583 2.573 1.00 0.00 C ATOM 478 H ILEA 36144.709 1.210 5.097 1.00 0.00 H ATOM **ATOM** 479 HA ILE A 36146.775 2.215 3.445 1.00 0.00 H 480 HB ILE A 36144.584 3.811 4.775 1.00 0.00 H ATOM ATOM 481 1HG1 ILE A 36144.560 2.354 2.122 1.00 0.00 H

482 2HG1 ILE A 36143.663 1.876 3.560 1.00 0.00 H ATOM 483 1HG2 ILE A 36146.620 4.385 2.734 1.00 0.00 H ATOM 484 2HG2 ILE A 36145.776 5.472 3.835 1.00 0.00 H ATOM 485 3HG2 ILE A 36144.989 4.936 2.351 1.00 0.00 H **ATOM** 486 1HD1 ILE A 36142.384 3.954 3.443 1.00 0.00 H **ATOM ATOM** 487 2HD1 ILE A 36142.225 2.999 1.970 1.00 0.00 H 488 3HD1 ILE A 36143.276 4.415 1.994 1.00 0.00 H ATOM 489 N ARGA 37148.276 3.661 4.804 1.00 0.00 N ATOM 490 CA ARGA 37149.245 4.367 5.633 1.00 0.00 C ATOM 491 C ARG A 37149.477 5.782 5.116 1.00 0.00 C ATOM **ATOM** 492 O ARG A 37149.185 6.761 5.804 1.00 0.00 O 493 CB ARG A 37150.569 3.602 5.672 1.00 0.00 C **ATOM** 494 CG ARGA 37150.404 2.115 5.937 1.00 0.00 C ATOM 495 CD ARG A 37150.291 1.823 7.424 1.00 0.00 C ATOM 496 NE ARG A 37149.079 2.397 8.006 1.00 0.00 N **ATOM ATOM** 497 CZ ARG A 37148.908 2.602 9.309 1.00 0.00 C 498 NH1 ARG A 37149.866 2.280 10.170 1.00 0.00 N **ATOM** 499 NH2 ARG A 37147.775 3.129 9.754 1.00 0.00 N **ATOM** 500 H ARGA 37148.478 3.510 3.857 1.00 0.00 H ATOM 501 HA ARG A 37148.844 4.424 6.635 1.00 0.00 H ATOM 502 1HB ARG A 37151.068 3.724 4.723 1.00 0.00 H ATOM ATOM 503 2HB ARG A 37151.188 4.018 6.452 1.00 0.00 H 504 1HG ARG A 37149.508 1.768 5.443 1.00 0.00 H **ATOM** 505 2HG ARG A 37151.261 1.592 5.540 1.00 0.00 H **ATOM** 506 1HD ARG A 37150.274 0.753 7.568 1.00 0.00 H **ATOM** 507 2HD ARG A 37151.152 2.240 7.926 1.00 0.00 H **ATOM ATOM** 508 HE ARGA 37148.356 2.643 7.392 1.00 0.00 H 509 1HH1 ARG A 37150.722 1.882 9.843 1.00 0.00 H ATOM 510 2HH1 ARG A 37149.730 2.437 11.149 1.00 0.00 H ATOM 511 1HH2 ARG A 37147.050 3.372 9.109 1.00 0.00 H ATOM 512 2HH2 ARG A 37147.646 3.282 10.734 1.00 0.00 H ATOM

513 N TRPA 38150.004 5.886 3.900 1.00 0.00 N ATOM 514 CA TRP A 38150.274 7.185 3.294 1.00 0.00 C ATOM 515 C TRPA 38149.557 7.323 1.954 1.00 0.00 C ATOM 516 O TRPA 38149.618 6.430 1.110 1.00 0.00 O **ATOM** 517 CB TRPA 38151.783 7.382 3.104 1.00 0.00 C ATOM 518 CG TRPA 38152.128 8.579 2.267 1.00 0.00 C ATOM ATOM 519 CD1 TRP A 38152.387 9.844 2.710 1.00 0.00 C 520 CD2 TRP A 38152.247 8.620 0.840 1.00 0.00 C ATOM **ATOM** 521 NE1 TRP A 38152.659 10.670 1.646 1.00 0.00 N 522 CE2 TRP A 38152.579 9.941 0.486 1.00 0.00 C **ATOM** 523 CE3 TRP A 38152.104 7.668 -0.174 1.00 0.00 C **ATOM** ATOM 524 CZ2 TRP A 38152.771 10.333 -0.836 1.00 0.00 C 525 CZ3 TRP A 38152.296 8.057 -1.486 1.00 0.00 C **ATOM** 526 CH2 TRP A 38152.625 9.380 -1.807 1.00 0.00 C ATOM **ATOM** 527 H TRPA 38150.216 5.071 3.400 1.00 0.00 H 528 HA TRP A 38149.904 7.945 3.964 1.00 0.00 H ATOM 529 1HB TRP A 38152.247 7.508 4.071 1.00 0.00 H **ATOM** 530 2HB TRP A 38152.195 6.507 2.623 1.00 0.00 H ATOM 531 HD1 TRP A 38152.376 10.139 3.748 1.00 0.00 H ATOM ATOM 532 HE1 TRP A 38152.875 11.623 1.706 1.00 0.00 H 533 HE3 TRP A 38151.850 6.644 0.055 1.00 0.00 H ATOM 534 HZ2 TRP A 38153.022 11.349 -1.102 1.00 0.00 H ATOM **ATOM** 535 HZ3 TRP A 38152.189 7.335 -2.281 1.00 0.00 H **ATOM** 536 HH2 TRP A 38152.765 9.638 -2.847 1.00 0.00 H 537 N ILE A 39148.889 8.456 1.765 1.00 0.00 N ATOM 538 CA ILE A 39148.169 8.727 0.528 1.00 0.00 C **ATOM** 539 C ILE A 39148.631 10.044 -0.083 1.00 0.00 C ATOM 540 O ILE A 39148.297 11.119 0.414 1.00 0.00 O ATOM 541 CB ILE A 39146.647 8.785 0.762 1.00 0.00 C ATOM 542 CG1 ILE A 39146.181 7.562 1.554 1.00 0.00 C **ATOM** 543 CG2 ILE A 39145.911 8.876 -0.567 1.00 0.00 C ATOM

544 CD1 ILE A 39144.818 7.736 2.187 1.00 0.00 C ATOM ATOM 545 H ILE A 39148.887 9.132 2.475 1.00 0.00 H 546 HA ILE A 39148.378 7.924 -0.165 1.00 0.00 H ATOM 547 HB ILE A 39146.427 9.678 1.328 1.00 0.00 H ATOM 548 1HG1 ILE A 39146.134 6.710 0.893 1.00 0.00 H ATOM ATOM 549 2HG1 ILE A 39146.891 7.360 2.342 1.00 0.00 H **ATOM** 550 1HG2 ILE A 39146.058 9.857 -0.994 1.00 0.00 H ATOM 551 2HG2 ILE A 39144.856 8.708 -0.405 1.00 0.00 H **ATOM** 552 3HG2 ILE A 39146.295 8.127 -1.243 1.00 0.00 H 553 1HD1 ILE A 39144.725 8.742 2.569 1.00 0.00 H **ATOM ATOM** 554 2HD1 ILE A 39144.706 7.032 2.998 1.00 0.00 H 555 3HD1 ILE A 39144.052 7.559 1.446 1.00 0.00 H **ATOM** 556 N GLY A 40149.407 9.955 -1.159 1.00 0.00 N ATOM 557 CA GLY A 40149.906 11.152 -1.808 1.00 0.00 C **ATOM ATOM** 558 C GLY A 40150.448 10.884 -3.197 1.00 0.00 C ATOM 559 O GLY A 40150.274 9.794 -3.742 1.00 0.00 O ATOM 560 H GLY A 40149.646 9.072 -1.510 1.00 0.00 H ATOM 561 1HA GLY A 40149.104 11.870 -1.880 1.00 0.00 H ATOM 562 2HA GLY A 40150.693 11.572 -1.202 1.00 0.00 H **ATOM** 563 N GLNA 41151.109 11.884 -3.769 1.00 0.00 N 564 CA GLN A 41151.683 11.763 -5.103 1.00 0.00 C ATOM **ATOM** 565 C GLN A 41153.162 12.148 -5.090 1.00 0.00 C 566 O GLN A 41153.506 13.302 -4.830 1.00 0.00 O **ATOM** 567 CB GLN A 41150.919 12.654 -6.082 1.00 0.00 C **ATOM** 568 CG GLN A 41149.411 12.488 -6.004 1.00 0.00 C **ATOM** 569 CD GLN A 41148.672 13.804 -6.138 1.00 0.00 C ATOM **ATOM** 570 OE1 GLN A 41148.635 14.607 -5.206 1.00 0.00 O **ATOM** 571 NE2 GLN A 41148.077 14.033 -7.304 1.00 0.00 N 572 H GLN A 41151.213 12.728 -3.282 1.00 0.00 H **ATOM** 573 HA GLN A 41151.588 10.735 -5.415 1.00 0.00 H **ATOM** 574 1HB GLN A 41151.157 13.685 -5.871 1.00 0:00 H ATOM

575 2HB GLN A 41151.235 12.418 -7.086 1.00 0.00 H 576 1HG GLN A 41149.090 11.832 -6.799 1.00 0.00 H ATOM 577 2HG GLN A 41149.158 12.046 -5.051 1.00 0.00 H **ATOM** 578 1HE2 GLN A 41148.148 13.349 -8.000 1.00 0.00 H **ATOM** 579 2HE2 GLN A 41147.594 14.878 -7.418 1.00 0.00 H ATOM **ATOM** 580 N PRO A 42154.062 11.187 -5.368 1.00 0.00 N 581 CA PRO A 42155.507 11.441 -5.381 1.00 0.00 C ATOM 582 C PRO A 42155.892 12.546 -6.360 1.00 0.00 C **ATOM** 583 O PRO A 42155.139 12.859 -7.283 1.00 0.00 O **ATOM** ATOM 584 CB PRO A 42156.107 10.102 -5.822 1.00 0.00 C **ATOM** 585 CG PRO A 42155.065 9.090 -5.491 1.00 0.00 C 586 CD PRO A 42153.749 9.784 -5.689 1.00 0.00 C ATOM 587 HA PRO A 42155.871 11.695 -4.396 1.00 0.00 H ATOM 588 1HB PRO A 42156.311 10.129 -6.882 1.00 0.00 H **ATOM** 589 2HB PRO A 42157.022 9.918 -5.279 1.00 0.00 H **ATOM ATOM** 590 1HG PRO A 42155.148 8.245 -6.157 1.00 0.00 H 591 2HG PRO A 42155.173 8.774 -4.464 1.00 0.00 H **ATOM** 592 1HD PRO A 42153.419 9.686 -6.713 1.00 0.00 H **ATOM** 593 2HD PRO A 42153.007 9.389 -5.010 1.00 0.00 H **ATOM** 594 N PRO A 43157.076 13.153 -6.172 1.00 0.00 N **ATOM** 595 CA PRO A 43157.559 14.227 -7.043 1.00 0.00 C ATOM **ATOM** 596 C PRO A 43157.974 13.715 -8.417 1.00 0.00 C 597 O PRO A 43159.140 13.389 -8.642 1.00 0.00 O **ATOM** 598 CB PRO A 43158.771 14.776 -6.291 1.00 0.00 C **ATOM** 599 CG PRO A 43159.256 13.633 -5.468 1.00 0.00 C **ATOM** 600 CD PRO A 43158.034 12.839 -5.096 1.00 0.00 C **ATOM ATOM** 601 HA PRO A 43156.820 15.006 -7.159 1.00 0.00 H 602 1HB PRO A 43159.519 15.100 -7.000 1.00 0.00 H ATOM 603 2HB PRO A 43158.469 15.608 -5.673 1.00 0.00 H ATOM 604 1HG PRO A 43159.935 13.027 -6.048 1.00 0.00 H **ATOM** 605 2HG PRO A 43159.747 14.004 -4.580 1.00 0.00 H ATOM

606 1HD PRO A 43158.262 11.783 -5.079 1.00 0.00 H 607 2HD PRO A 43157.654 13.158 -4.137 1.00 0.00 H **ATOM** 608 N GLY A 44157.015 13.646 -9.332 1.00 0.00 N ATOM 609 CA GLY A 44157.304 13.172 -10.672 1.00 0.00 C ATOM 610 C GLY A 44156.071 12.647 -11.380 1.00 0.00 C ATOM 611 O GLY A 44155.783 13.041 -12.510 1.00 0.00 O ATOM 612 H GLY A 44156.104 13.919 -9.097 1.00 0.00 H 613 1HA GLY A 44157.716 13.985 -11.248 1.00 0.00 H ATOM 614 2HA GLY A 44158.035 12.380 -10.612 1.00 0.00 H ATOM 615 N LEUA 45155.344 11.756 -10.716 1.00 0.00 N ATOM 616 CA LEUA 45154.136 11.177 -11.291 1.00 0.00 C 617 C LEUA 45152.926 11.462 -10.410 1.00 0.00 C ATOM 618 O LEUA 45152.826 10.948 -9.296 1.00 0.00 O **ATOM** 619 CB LEUA 45154.307 9.668 -11.472 1.00 0.00 C **ATOM** 620 CG LEUA 45154.840 8.927 -10.245 1.00 0.00 C ATOM 621 CD1 LEU A 45154.467 7.451 -10.307 1.00 0.00 C ATOM 622 CD2 LEU A 45156.350 9.096 -10.132 1.00 0.00 C **ATOM** 623 H LEUA 45155.624 11.483 -9.816 1.00 0.00 H ATOM 624 HA LEUA 45153.977 11.632 -12.258 1.00 0.00 H ATOM **ATOM** 625 1HB LEU A 45153.346 9.248 -11.733 1.00 0.00 H 626 2HB LEU A 45154.989 9.500 -12.292 1.00 0.00 H ATOM 627 HG LEUA 45154.389 9.345 -9.357 1.00 0.00 H **ATOM** 628 1HD1 LEU A 45153.870 7.266 -11.188 1.00 0.00 H ATOM 629 2HD1 LEU A 45153.901 7.186 -9.427 1.00 0.00 H **ATOM** 630 3HD1 LEU A 45155.365 6.852 -10.350 1.00 0.00 H **ATOM** 631 1HD2 LEU A 45156.683 9.843 -10.837 1.00 0.00 H ATOM 632 2HD2 LEU A 45156.836 8.157 -10.349 1.00 0.00 H ATOM ATOM 633 3HD2 LEU A 45156.602 9.408 -9.130 1.00 0.00 H 634 N ASNA 46152.008 12.282 -10.911 1.00 0.00 N ATOM 635 CA ASN A 46150.810 12.622 -10.156 1.00 0.00 C **ATOM** ATOM 636 C ASN A 46149.846 11.443 -10.124 1.00 0.00 C

ATOM 637 O ASN A 46149.218 11.110 -11.130 1.00 0.00 O 638 CB ASN A 46150.123 13.843 -10.773 1.00 0.00 C ATOM ATOM 639 CG ASN A 46149.380 14.670 -9.743 1.00 0.00 C 640 OD1 ASN A 46149.955 15.100 -8.743 1.00 0.00 O ATOM **ATOM** 641 ND2 ASN A 46148.095 14.900 -9.984 1.00 0.00 N ATOM 642 H ASN A 46152.139 12.664 -11.804 1.00 0.00 H 643 HA ASN A 46151.108 12.858 -9.146 1.00 0.00 H ATOM 644 1HB ASN A 46150.868 14.469 -11.241 1.00 0.00 H ATOM 645 2HB ASN A 46149.417 13.511 -11.519 1.00 0.00 H ATOM ATOM 646 1HD2 ASN A 46147.703 14.526 -10.801 1.00 0.00 H 647 2HD2 ASN A 46147.590 15.433 -9.335 1.00 0.00 H ATOM 648 N GLUA 47149.734 10.813 -8.961 1.00 0.00 N ATOM 649 CA GLUA 47148.848 9.668 -8.790 1.00 0.00 C ATOM 650 C GLUA 47148.661 9.345 -7.312 1.00 0.00 C ATOM ATOM 651 O GLUA 47149.627 9.062 -6.604 1.00 0.00 O **ATOM** 652 CB GLU A 47149.405 8.446 -9.525 1.00 0.00 C 653 CG GLU A 47150.918 8.314 -9.439 1.00 0.00 C ATOM 654 CD GLUA 47151.479 7.357 -10.472 1.00 0.00 C **ATOM** 655 OE1 GLU A 47151.460 7.702 -11.672 1.00 0.00 O ATOM 656 OE2 GLU A 47151.937 6.263 -10.082 1.00 0.00 O ATOM ATOM 657 H GLUA 47150,262 11.125 -8.197 1.00 0.00 H 658 HA GLUA 47147.889 9.926 -9.214 1.00 0.00 H ATOM 659 1HB GLU A 47148,964 7.555 -9.103 1.00 0.00 H ATOM 660 2HB GLU A 47149.131 8.513 -10.568 1.00 0.00 H **ATOM** 661 1HG GLU A 47151.360 9.285 -9.592 1.00 0.00 H **ATOM** 662 2HG GLUA 47151.180 7.952 -8.455 1.00 0.00 H ATOM 663 N VALA 48147.416 9.382 -6.851 1.00 0.00 N ATOM 664 CA VALA 48147.116 9.085 -5.457 1.00 0.00 C **ATOM ATOM** 665 C VALA 48147.475 7.642 -5.124 1.00 0.00 C 666 O VALA 48146.726 6.717 -5.438 1.00 0.00 O **ATOM** 667 CB VALA 48145.629 9.320 -5.137 1.00 0.00 C **ATOM**

668 CG1 VAL A 48145.378 9.198 -3.642 1.00 0.00 C ATOM 669 CG2 VAL A 48145.180 10.679 -5.652 1.00 0.00 C ATOM **ATOM** 670 H VALA 48146.684 9.609 -7.462 1.00 0.00 H 671 HA VALA 48147.709 9.745 -4.840 1.00 0.00 H ATOM **ATOM** 672 HB VALA 48145.048 8.560 -5.639 1.00 0.00 H 673 1HG1 VALA 48144.420 9.634 -3.401 1.00 0.00 H ATOM 674 2HG1 VALA 48146.156 9.719 -3.103 1.00 0.00 H ATOM 675 3HG1 VAL A 48145.381 8.155 -3.360 1.00 0.00 H **ATOM** 676 1HG2 VAL A 48144.227 10.934 -5.213 1.00 0.00 H ATOM ATOM 677 2HG2 VAL A 48145.083 10.644 -6.726 1.00 0.00 H 678 3HG2 VAL A 48145.912 11.426 -5.381 1.00 0.00 H ATOM 679 N LEUA 49148.629 7.455 -4.492 1.00 0.00 N ATOM 680 CA LEU A 49149.088 6.123 -4.122 1.00 0.00 C ATOM 681 C LEUA 49148.955 5.904 -2.621 1.00 0.00 C ATOM 682 O LEUA 49149.633 6.554 -1.825 1.00 0.00 O **ATOM** ATOM 683 CB LEU A 49150.544 5.923 -4.550 1.00 0.00 C 684 CG LEUA 49150.801 6.069 -6.051 1.00 0.00 C ATOM 685 CD1 LEU A 49152.275 6.335 -6.317 1.00 0.00 C **ATOM** 686 CD2 LEU A 49150.342 4.822 -6.793 1.00 0.00 C ATOM 687 H LEUA 49149.185 8.231 -4.270 1.00 0.00 H **ATOM ATOM** 688 HA LEU A 49148.470 5.404 -4.636 1.00 0.00 H **ATOM** 689 1HB LEU A 49151.153 6.649 -4.030 1.00 0.00 H 690 2HB LEU A 49150.854 4.935 -4.249 1.00 0.00 H **ATOM** 691 HG LEU A 49150.237 6.910 -6.427 1.00 0.00 H **ATOM** 692 1HD1 LEU A 49152.707 6.843 -5.468 1.00 0.00 H **ATOM** 693 2HD1 LEU A 49152.376 6.954 -7.197 1.00 0.00 H **ATOM** 694 3HD1 LEU A 49152.788 5.398 -6.475 1.00 0.00 H ATOM 695 1HD2 LEU A 49151.185 4.165 -6.951 1.00 0.00 H ATOM **ATOM** 696 2HD2 LEU A 49149.921 5.104 -7.746 1.00 0.00 H 697 3HD2 LEU A 49149.593 4.311 -6.206 1.00 0.00 H ATOM 698 N ALAA 50148.077 4.984 -2.240 1.00 0.00 N

ATOM 699 CA ALA A 50147.856 4.682 -0.832 1.00 0.00 C 700 C ALAA 50148.756 3.542 -0.369 1.00 0.00 C **ATOM** 701 O ALAA 50148.624 2.408 -0.830 1.00 0.00 O **ATOM ATOM** 702 CB ALA A 50146.395 4.337 -0.589 1.00 0.00 C 703 H ALAA 50147.565 4.497 -2.920 1.00 0.00 H **ATOM ATOM** 704 HA ALAA 50148.093 5.570 -0.265 1.00 0.00 H 705 1HB ALA A 50145.792 4.740 -1.389 1.00 0.00 H **ATOM ATOM** 706 2HB ALA A 50146.077 4.763 0.352 1.00 0.00 H 707 3HB ALA A 50146.278 3.265 -0.556 1.00 0.00 H **ATOM** ATOM 708 N GLY A 51149.671 3.850 0.545 1.00 0.00 N **ATOM** 709 CA GLY A 51150.578 2.839 1.056 1.00 0.00 C 710 C GLY A 51149.878 1.821 1.933 1.00 0.00 C **ATOM** 711 O GLY A 51149.350 2.162 2.991 1.00 0.00 O **ATOM ATOM** 712 H GLY A 51149.730 4.770 0.876 1.00 0.00 H 713 1HA GLY A 51151.034 2.326 0.221 1.00 0.00 H **ATOM ATOM** 714 2HA GLY A 51151.352 3.324 1.631 1.00 0.00 H 715 N LEUA 52149.873 0.567 1.494 1.00 0.00 N **ATOM** 716 CA LEUA 52149.232 -0.504 2.247 1.00 0.00 C **ATOM** 717 C LEUA 52150.270 -1.379 2.943 1.00 0.00 C **ATOM** 718 O LEUA 52151.305 -1.710 2.364 1.00 0.00 O **ATOM ATOM** 719 CB LEU A 52148.365 -1.360 1.322 1.00 0.00 C **ATOM** 720 CG LEU A 52147.140 -0.650 0.742 1.00 0.00 C 721 CD1 LEU A 52146.534 -1.469 -0.388 1.00 0.00 C ATOM 722 CD2 LEU A 52146.108 -0.394 1.830 1.00 0.00 C **ATOM** 723 H LEUA 52150.311 0.356 0.643 1.00 0.00 H **ATOM** 724 HA LEUA 52148.601 -0.050 2.997 1.00 0.00 H **ATOM** 725 1HB LEU A 52148.980 -1.701 0.501 1.00 0.00 H ATOM 726 2HB LEU A 52148.024 -2.221 1.876 1.00 0.00 H **ATOM ATOM** 727 HG LEU A 52147.444 0.305 0.336 1.00 0.00 H 728 1HD1 LEU A 52145.929 -0.828 -1.012 1.00 0.00 H **ATOM** 729 2HD1 LEU A 52145.918 -2.253 0.027 1.00 0.00 H ATOM

ATOM 730 3HD1 LEU A 52147.324 -1.906 -0.979 1.00 0.00 H 731 1HD2 LEU A 52146.587 0.078 2.675 1.00 0.00 H **ATOM** 732 2HD2 LEU A 52145.673 -1.332 2.141 1.00 0.00 H **ATOM** 733 3HD2 LEU A 52145.334 0.254 1.447 1.00 0.00 H ATOM **ATOM** 734 N GLUA 53149.985 -1.750 4.187 1.00 0.00 N ATOM 735 CA GLU A 53150.892 -2.587 4.962 1.00 0.00 C 736 C GLUA 53150.367 -4.015 5.058 1.00 0.00 C **ATOM** 737 O GLUA 53149.392 -4.282 5.759 1.00 0.00 O ATOM 738 CB GLU A 53151.084 -2.006 6.365 1.00 0.00 C ATOM ATOM 739 CG GLU A 53152.053 -2.799 7.225 1.00 0.00 C 740 CD GLUA 53151.694 -2.758 8.697 1.00 0.00 C **ATOM** 741 OE1 GLU A 53152.597 -2.965 9.535 1.00 0.00 O **ATOM** 742 OE2 GLU A 53150.510 -2.518 9.013 1.00 0.00 O **ATOM** 743 H GLUA 53149.143 -1.454 4.594 1.00 0.00 H **ATOM** 744 HA GLUA 53151.846 -2.599 4.455 1.00 0.00 H ATOM **ATOM** 745 1HB GLU A 53151.457 -0.996 6.276 1.00 0.00 H 746 2HB GLU A 53150.127 -1.982 6.865 1.00 0.00 H ATOM 747 1HG GLUA 53152.046 -3.828 6.898 1.00 0.00 H **ATOM** 748 2HG GLUA 53153.045 -2.389 7.100 1.00 0.00 H **ATOM** 749 N LEUA 54151.021 -4.929 4.348 1.00 0.00 N **ATOM** ATOM 750 CA LEU A 54150.618 -6.331 4.353 1.00 0.00 C **ATOM** 751 C LEUA 54150.983 -6.997 5.676 1.00 0.00 C 752 O LEUA 54152.069 -6.783 6.212 1.00 0.00 O ATOM 753 CB LEU A 54151.282 -7.078 3.194 1.00 0.00 C **ATOM** 754 CG LEUA 54151.184 -6.382 1.835 1.00 0.00 C **ATOM** 755 CD1 LEU A 54152.187 -6.976 0.859 1.00 0.00 C **ATOM** 756 CD2 LEU A 54149.771 -6.491 1.283 1.00 0.00 C **ATOM** 757 H LEUA 54151.791 -4.655 3.808 1.00 0.00 H **ATOM ATOM** 758 HA LEU A 54149.547 -6.369 4.227 1.00 0.00 H 759 1HB LEUA 54152.327 -7.213 3.433 1.00 0.00 H **ATOM** 760 2HB LEUA 54150.821 -8.050 3.109 1.00 0.00 H

761 HG LEU A 54151.417 -5.334 1.957 1.00 0.00 H ATOM 762 1HD1 LEU A 54151.706 -7.745 0.272 1.00 0.00 H ATOM 763 2HD1 LEU A 54153.012 -7.406 1.407 1.00 0.00 H ATOM 764 3HD1 LEU A 54152.555 -6.200 0.205 1.00 0.00 H **ATOM** 765 1HD2 LEU A 54149.795 -6.380 0.209 1.00 0.00 H **ATOM ATOM** 766 2HD2 LEU A 54149.156 -5.713 1.712 1.00 0.00 H 767 3HD2 LEU A 54149.359 -7.457 1.536 1.00 0.00 H **ATOM** 768 N GLUA 55150.065 -7.806 6.197 1.00 0.00 N **ATOM** 769 CA GLU A 55150.290 -8.504 7.458 1.00 0.00 C **ATOM** 770 C GLUA 55151.347 -9.593 7.295 1.00 0.00 C **ATOM ATOM** 771 O GLUA 55152.090 -9.894 8.229 1.00 0.00 O 772 CB GLU A 55148.983 -9.117 7.965 1.00 0.00 C ATOM 773 CG GLU A 55147.843 -8.118 8.067 1.00 0.00 C **ATOM** 774 CD GLUA 55147.017 -8.302 9.326 1.00 0.00 C ATOM 775 OE1 GLU A 55147.071 -9.401 9.916 1.00 0.00 O **ATOM ATOM** 776 OE2 GLU A 55146.318 -7.346 9.722 1.00 0.00 O 777 H GLUA 55149.218 -7.937 5.723 1.00 0.00 H ATOM 778 HA GLU A 55150.642 -7.782 8.179 1.00 0.00 H **ATOM** 779 1HB GLU A 55148.683 -9.906 7.291 1.00 0.00 H ATOM 780 2HB GLU A 55149.154 -9.538 8.945 1.00 0.00 H **ATOM** 781 1HG GLU A 55148.254 -7.120 8.069 1.00 0.00 H ATOM 782 2HG GLU A 55147.198 -8.239 7.210 1.00 0.00 H **ATOM** 783 N ASPA 56151.406 -10.179 6.103 1.00 0.00 N ATOM 784 CA ASP A 56152.372 -11.234 5.818 1.00 0.00 C **ATOM** 785 C ASP A 56153.664 -10.651 5.256 1.00 0.00 C **ATOM** 786 O ASPA 56153.650 -9.931 4.258 1.00 0.00 O **ATOM** 787 CB ASP A 56151.781 -12.241 4.830 1.00 0.00 C ATOM 788 CG ASP A 56150.691 -13.091 5.453 1.00 0.00 C ATOM 789 OD1 ASP A 56149.769 -13.504 4.718 1.00 0.00 O **ATOM** 790 OD2 ASP A 56150.759 -13.342 6.674 1.00 0.00 O **ATOM** 791 H ASPA 56150.786 -9.895 5.399 1.00 0.00 H ATOM

792 HA ASPA 56152.593 -11.741 6.745 1.00 0.00 H ATOM 793 1HB ASP A 56151.362 -11.708 3.990 1.00 0.00 H ATOM 794 2HB ASP A 56152.566 -12.895 4.480 1.00 0.00 H **ATOM** 795 N GLUA 57154.781 -10.966 5.905 1.00 0.00 N **ATOM** 796 CA GLU A 57156.083 -10.474 5.470 1.00 0.00 C **ATOM ATOM** 797 C GLUA 57156.427 -10.999 4.080 1.00 0.00 C 798 O GLUA 57156.851 -12.145 3.927 1.00 0.00 O **ATOM** 799 CB GLUA 57157.167 -10.886 6.467 1.00 0.00 C **ATOM** 800 CG GLU A 57157.113 -10.116 7.776 1.00 0.00 C **ATOM** 801 CD GLUA 57157.985 -10.733 8.852 1.00 0.00 C **ATOM** 802 OE1 GLU A 57158.567 -9.973 9.653 1.00 0.00 O **ATOM** 803 OE2 GLU A 57158.086 -11.977 8.892 1.00 0.00 O **ATOM** 804 H GLUA 57154.728 -11.545 6.694 1.00 0.00 H **ATOM** 805 HA GLUA 57156.033 -9.396 5.431 1.00 0.00 H **ATOM** 806 1HB GLUA 57157.056 -11.937 6.687 1.00 0.00 H ATOM 807 2HB GLU A 57158.135 -10.721 6.017 1.00 0.00 H ATOM 808 1HG GLU A 57157.448 -9.105 7.599 1.00 0.00 H **ATOM** 809 2HG GLU A 57156.092 -10.099 8.127 1.00 0.00 H ATOM 810 N CYS A 58156.242 -10.156 3.070 1.00 0.00 N ATOM 811 CA CYS A 58156.533 -10.535 1.693 1.00 0.00 C **ATOM** 812 C CYS A 58157.946 -10.114 1.300 1.00 0.00 C ATOM **ATOM** 813 O CYS A 58158.303 -8.939 1.397 1.00 0.00 O 814 CB CYS A 58155.516 -9.904 0.742 1.00 0.00 C ATOM 815 SG CYS A 58154.053 -10.924 0.443 1.00 0.00 S ATOM 816 H CYS A 58155.901 -9.256 3.256 1.00 0.00 H **ATOM** 817 HA CYS A 58156.460 -11.611 1.623 1.00 0.00 H ATOM 818 1HB CYS A 58155.181 -8.965 1.156 1.00 0.00 H ATOM ATOM 819 2HB CYS A 58155.991 -9.722 -0.212 1.00 0.00 H ATOM 820 HG CYS A 58153.934 -10.999 -0.506 1.00 0.00 H 821 N ALAA 59158.744 -11.079 0.855 1.00 0.00 N ATOM ATOM 822 CA ALA A 59160.117 -10.807 0.448 1.00 0.00 C

- ATOM 823 C ALAA 59160.156 -9.970 -0.826 1.00 0.00 C
 ATOM 824 O ALAA 59159.813 -10.450 -1.907 1.00 0.00 O
- ATOM 825 CB ALAA 59160.876 -12.111 0.249 1.00 0.00 C
- ATOM 826 H ALAA 59158.402 -11.995 0.801 1.00 0.00 H
- ATOM 827 HA ALA A 59160.598 -10.256 1.243 1.00 0.00 H
- ATOM 828 1HB ALA A 59160.889 -12.363 -0.801 1.00 0.00 H
- ATOM 829 2HB ALA A 59160.387 -12.900 0.802 1.00 0.00 H
- ATOM 830 3HB ALA A 59161.889 -11.995 0.605 1.00 0.00 H
- ATOM 831 N GLY A 60160.576 -8.716 -0.692 1.00 0.00 N
- ATOM 832 CA GLY A 60160.651 -7.832 -1.840 1.00 0.00 C
- ATOM 833 C GLY A 60160.053 -6.468 -1.563 1.00 0.00 C
- ATOM 834 O GLY A 60160.466 -5.470 -2.152 1.00 0.00 O
- ATOM 835 H GLY A 60160.836 -8.388 0.194 1.00 0.00 H
- ATOM 836 1HA GLY A 60161.688 -7.708 -2.117 1.00 0.00 H
- ATOM 837 2HA GLY A 60160.122 -8.286 -2.665 1.00 0.00 H
- ATOM 838 N CYS A 61159.074 -6.425 -0.664 1.00 0.00 N
- ATOM 839 CA CYS A 61158.416 -5.173 -0.311 1.00 0.00 C
- ATOM 840 C CYS A 61159.344 -4.284 0.510 1.00 0.00 C
- ATOM 841 O CYS A 61160.455 -4.683 0.860 1.00 0.00 O
- ATOM 842 CB CYS A 61157.132 -5.451 0.472 1.00 0.00 C
- ATOM 843 SG CYS A 61156.021 -6.631 -0.329 1.00 0.00 S
- ATOM 844 H CYS A 61158.788 -7.255 -0.229 1.00 0.00 H
- ATOM 845 HA CYS A 61158.164 -4.661 -1.227 1.00 0.00 H
- ATOM 846 1HB CYS A 61157.389 -5.850 1.442 1.00 0.00 H
- ATOM 847 2HB CYS A 61156.591 -4.525 0.602 1.00 0.00 H
- ATOM 848 HG CYS A 61155.639 -7.189 0.354 1.00 0.00 H
- ATOM 849 N THR A 62158.881 -3.076 0.816 1.00 0.00 N
- ATOM 850 CA THR A 62159.669 -2.129 1.596 1.00 0.00 C
- ATOM 851 C THR A 62159.163 -2.056 3.034 1.00 0.00 C
- ATOM 852 O THR A 62158.177 -2.701 3.389 1.00 0.00 O
- ATOM 853 CB THR A 62159.619 -0.742 0.955 1.00 0.00 C

854 OG1 THR A 62158.314 -0.454 0.483 1.00 0.00 O **ATOM** 855 CG2 THR A 62160.573 -0.585 -0.208 1.00 0.00 C **ATOM** 856 H THR A 62157.987 -2.815 0.509 1.00 0.00 H **ATOM** 857 HA THR A 62160.691 -2.476 1.603 1.00 0.00 H **ATOM ATOM** 858 HB THR A 62159.881 -0.003 1.699 1.00 0.00 H 859 HG1 THR A 62157.782 -0.107 1.204 1.00 0.00 H ATOM 860 1HG2 THR A 62160.889 -1.560 -0.549 1.00 0.00 H **ATOM** 861 2HG2 THR A 62161.435 -0.018 0.108 1.00 0.00 H ATOM **ATOM** 862 3HG2 THR A 62160.076 -0.066 -1.014 1.00 0.00 H **ATOM** 863 N ASPA 63159.847 -1.268 3.857 1.00 0.00 N 864 CA ASPA 63159.467 -1.109 5.255 1.00 0.00 C ATOM **ATOM** 865 C ASPA 63158.836 0.257 5.497 1.00 0.00 C 866 O ASPA 63158.965 0.829 6.578 1.00 0.00 O **ATOM** 867 CB ASPA 63160.689 -1.287 6.160 1.00 0.00 C ATOM 868 CG ASPA 63161.787 -0.290 5.849 1.00 0.00 C **ATOM** 869 OD1 ASP A 63162.647 -0.600 4.998 1.00 0.00 O **ATOM** 870 OD2 ASP A 63161.789 0.801 6.458 1.00 0.00 O **ATOM** 871 H ASPA 63160.625 -0.779 3.514 1.00 0.00 H **ATOM** 872 HA ASPA 63158.743 -1.875 5.490 1.00 0.00 H **ATOM** 873 1HB ASPA 63160.388 -1.156 7.188 1.00 0.00 H **ATOM** 874 2HB ASP A 63161.083 -2.284 6.029 1.00 0.00 H **ATOM** 875 N GLY A 64158.152 0.775 4.482 1.00 0.00 N **ATOM** 876 CA GLY A 64157.511 2.071 4.603 1.00 0.00 C **ATOM** 877 C GLYA 64158.215 3.146 3.799 1.00 0.00 C **ATOM** 878 O GLY A 64158.375 4.274 4.263 1.00 0.00 O ATOM 879 H GLY A 64158.083 0.274 3.642 1.00 0.00 H ATOM 880 1HA GLY A 64156.490 1.989 4.257 1.00 0.00 H ATOM 881 2HA GLY A 64157.505 2.362 5.643 1.00 0.00 H ATOM 882 N THR A 65158.638 2.795 2.589 1.00 0.00 N **ATOM** 883 CA THR A 65159.329 3.737 1.717 1.00 0.00 C ATOM 884 C THR A 65158.943 3.515 0.260 1.00 0.00 C ATOM

885 O THR A 65159.044 2.402 -0.257 1.00 0.00 O ATOM 886 CB THR A 65160.844 3.600 1.884 1.00 0.00 C ATOM 887 OG1 THR A 65161.250 2.258 1.686 1.00 0.00 O ATOM 888 CG2 THR A 65161.338 4.034 3.246 1.00 0.00 C **ATOM** 889 H THR A 65158.481 1.880 2.275 1.00 0.00 H ATOM 890 HA THR A 65159.034 4.734 2.008 1.00 0.00 H ATOM ATOM 891 HB THR A 65161.334 4.215 1.143 1.00 0.00 H 892 HG1 THR A 65160.827 1.907 0.900 1.00 0.00 H ATOM **ATOM** 893 1HG2 THR A 65160.554 4.569 3.761 1.00 0.00 H 894 2HG2 THR A 65162.197 4.679 3.129 1.00 0.00 H **ATOM** 895 3HG2 THR A 65161.619 3.164 3.822 1.00 0.00 H **ATOM** ATOM 896 N PHE A 66158.503 4.581 -0.399 1.00 0.00 N 897 CA PHE A 66158.101 4.504 -1.799 1.00 0.00 C **ATOM** 898 C PHE A 66159.101 5.230 -2.694 1.00 0.00 C ATOM 899 O PHE A 66159.198 6.457 -2.665 1.00 0.00 O **ATOM** 900 CB PHE A 66156.705 5.101 -1.985 1.00 0.00 C ATOM 901 CG PHE A 66156.083 4.770 -3.311 1.00 0.00 C **ATOM** 902 CD1 PHE A 66155.689 5.778 -4.177 1.00 0.00 C **ATOM** 903 CD2 PHE A 66155.893 3.452 -3.692 1.00 0.00 C ATOM **ATOM** 904 CE1 PHE A 66155.116 5.476 -5.398 1.00 0.00 C 905 CE2 PHE A 66155.321 3.144 -4.912 1.00 0.00 C **ATOM ATOM** 906 CZ PHE A 66154.932 4.158 -5.766 1.00 0.00 C 907 H PHE A 66158.446 5.442 0.066 1.00 0.00 H **ATOM** 908 HA PHE A 66158.077 3.461 -2.080 1.00 0.00 H **ATOM** 909 1HB PHE A 66156.055 4.726 -1.211 1.00 0.00 H **ATOM** 910 2HB PHE A 66156.768 6.176 -1.906 1.00 0.00 H ATOM 911 HD1 PHE A 66155.833 6.809 -3.891 1.00 0.00 H **ATOM** 912 HD2 PHE A 66156.196 2.659 -3.026 1.00 0.00 H ATOM 913 HE1 PHE A 66154.813 6.271 -6.064 1.00 0.00 H ATOM 914 HE2 PHE A 66155.178 2.112 -5.197 1.00 0.00 H ATOM ATOM 915 HZ PHE A 66154.485 3.919 -6.720 1.00 0.00 H

916 N ARG A 67159.843 4.465 -3.487 1.00 0.00 N **ATOM ATOM** 917 CA ARG A 67160.835 5.035 -4.390 1.00 0.00 C 918 C ARGA 67161.898 5.807 -3.615 1.00 0.00 C **ATOM ATOM** 919 O ARG A 67162.370 6.853 -4.062 1.00 0.00 O **ATOM** 920 CB ARG A 67160.158 5,956 -5.408 1.00 0.00 C 921 CG ARG A 67158.907 5.359 -6.030 1.00 0.00 C **ATOM** 922 CD ARG A 67158.567 6.031 -7.350 1.00 0.00 C ATOM **ATOM** 923 NE ARG A 67157.502 5.330 -8.063 1.00 0.00 N **ATOM** 924 CZ ARG A 67157.666 4.161 -8.677 1.00 0.00 C 925 NH1 ARG A 67158.849 3.558 -8.668 1.00 0.00 N **ATOM ATOM** 926 NH2 ARG A 67156.644 3.591 -9.302 1.00 0.00 N 927 H ARG A 67159.719 3.493 -3.465 1.00 0.00 H ATOM **ATOM** 928 HA ARG A 67161.311 4.220 -4.917 1.00 0.00 H 929 1HB ARG A 67159.886 6.877 -4.916 1.00 0.00 H **ATOM** 930 2HB ARG A 67160.859 6.174 -6.199 1.00 0.00 H ATOM 931 1HG ARG A 67159.071 4.306 -6.206 1.00 0.00 H **ATOM** 932 2HG ARG A 67158.080 5.488 -5.346 1.00 0.00 H **ATOM ATOM** 933 1HD ARG A 67158.248 7.043 -7.152 1.00 0.00 H 934 2HD ARG A 67159.452 6.048 -7.969 1.00 0.00 H **ATOM** 935 HE ARG A 67156.618 5.753 -8.086 1.00 0.00 H **ATOM** 936 1HH1 ARG A 67159.623 3.982 -8.199 1.00 0.00 H **ATOM** 937 2HH1 ARG A 67158.966 2.679 -9.131 1.00 0.00 H ATOM ATOM 938 1HH2 ARG A 67155.752 4.040 -9.312 1.00 0.00 H 939 2HH2 ARG A 67156.767 2.712 -9.763 1.00 0.00 H ATOM 940 N GLY A 68162.269 5.284 -2.451 1.00 0.00 N ATOM 941 CA GLY A 68163.274 5.938 -1.632 1.00 0.00 C **ATOM** 942 C GLY A 68162.724 7.136 -0.883 1.00 0.00 C ATOM 943 O GLY A 68163.458 8.076 -0.580 1.00 0.00 O **ATOM** 944 H GLY A 68161.859 4.449 -2.145 1.00 0.00 H **ATOM** 945 1HA GLY A 68163.658 5.225 -0.917 1.00 0.00 H **ATOM** ATOM 946 2HA GLY A 68164.084 6.265 -2.268 1.00 0.00 H

947 N THR A 69161.430 7.102 -0.584 1.00 0.00 N ATOM 948 CA THR A 69160.783 8.193 0.133 1.00 0.00 C ATOM **ATOM** 949 C THR A 69159.899 7.658 1.256 1.00 0.00 C 950 O THR A 69158.746 7.291 1.030 1.00 0.00 O ATOM **ATOM** 951 CB THR A 69159.948 9.040 -0.828 1.00 0.00 C 952 OG1 THR A 69160.661 9.285 -2.028 1.00 0.00 O **ATOM** 953 CG2 THR A 69159.546 10.380 -0.251 1.00 0.00 C **ATOM** 954 H THR A 69160.897 6.324 -0.852 1.00 0.00 H ATOM 955 HA THR A 69161.556 8.811 0.565 1.00 0.00 H ATOM 956 HB THR A 69159.044 8.501 -1.074 1.00 0.00 H **ATOM** 957 HG1 THR A 69160.425 8.623 -2.681 1.00 0.00 H ATOM **ATOM** 958 1HG2 THR A 69159.640 11.143 -1.010 1.00 0.00 H 959 2HG2 THR A 69160.189 10.619 0.583 1.00 0.00 H ATOM 960 3HG2 THR A 69158.521 10.334 0.087 1.00 0.00 H ATOM 961 N ARGA 70160.448 7.616 2.465 1.00 0.00 N ATOM 962 CA ARG A 70159.709 7.125 3.623 1.00 0.00 C **ATOM** 963 C ARG A 70158.552 8.058 3.966 1.00 0.00 C **ATOM** 964 O ARG A 70158.739 9.263 4.126 1.00 0.00 O **ATOM** 965 CB ARG A 70160.641 6.985 4.828 1.00 0.00 C **ATOM** 966 CG ARG A 70159.945 6.478 6.082 1.00 0.00 C **ATOM** 967 CD ARG A 70159.718 7.595 7.090 1.00 0.00 C **ATOM** 968 NE ARG A 70160.355 7.311 8.373 1.00 0.00 N **ATOM** 969 CZ ARG A 70161.654 7.482 8.610 1.00 0.00 C **ATOM** 970 NH1 ARG A 70162.457 7.933 7.653 1.00 0.00 N **ATOM** 971 NH2 ARG A 70162.152 7.201 9.806 1.00 0.00 N ATOM 972 H ARG A 70161.371 7.922 2.583 1.00 0.00 H **ATOM** 973 HA ARG A 70159.310 6.153 3.374 1.00 0.00 H ATOM 974 1HB ARG A 70161.433 6.293 4.577 1.00 0.00 H ATOM 975 2HB ARG A 70161.075 7.949 5.046 1.00 0.00 H **ATOM** 976 1HG ARGA 70158.990 6.057 5.806 1.00 0.00 H ATOM ATOM 977 2HG ARG A 70160.558 5.714 6.537 1.00 0.00 H

978 1HD ARG A 70160.124 8.513 6.692 1.00 0.00 H **ATOM** 979 2HD ARG A 70158.654 7.709 7.245 1.00 0.00 H **ATOM ATOM** 980 HE ARG A 70159.786 6.977 9.097 1.00 0.00 H 981 1HH1 ARG A 70162.087 8.147 6.749 1.00 0.00 H **ATOM ATOM** 982 2HH1 ARG A 70163.431 8.058 7.838 1.00 0.00 H 983 1HH2 ARG A 70161.552 6.861 10.530 1.00 0.00 H ATOM 984 2HH2 ARG A 70163.127 7.329 9.983 1.00 0.00 H ATOM 985 N TYR A 71157.355 7.490 4.077 1.00 0.00 N ATOM 986 CA TYR A 71156.166 8.269 4.402 1.00 0.00 C ATOM ATOM 987 C TYR A 71155.674 7.950 5.809 1.00 0.00 C 988 O TYR A 71155.102 8.804 6.486 1.00 0.00 O ATOM 989 CB TYR A 71155.057 7.991 3.386 1.00 0.00 C **ATOM** 990 CG TYR A 71155.312 8.601 2.026 1.00 0.00 C **ATOM** 991 CD1 TYR A 71155.252 7.827 0.874 1.00 0.00 C **ATOM ATOM** 992 CD2 TYR A 71155.614 9.951 1.894 1.00 0.00 C **ATOM** 993 CE1 TYR A 71155.486 8.380 -0.370 1.00 0.00 C 994 CE2 TYR A 71155.847 10.512 0.653 1.00 0.00 C ATOM 995 CZ TYR A 71155.783 9.722 -0.476 1.00 0.00 C **ATOM** 996 OH TYR A 71156.016 10.276 -1.713 1.00 0.00 O **ATOM** 997 H TYR A 71157.270 6.524 3.937 1.00 0.00 H ATOM 998 HA TYR A 71156.431 9.314 4.354 1.00 0.00 H ATOM 999 1HB TYR A 71154.956 6.924 3.256 1.00 0.00 H **ATOM** ATOM 1000 2HB TYR A 71154.126 8.393 3.761 1.00 0.00 H ATOM 1001 HD1 TYR A 71155.020 6.775 0.960 1.00 0.00 H ATOM 1002 HD2 TYR A 71155.664 10.567 2.780 1.00 0.00 H ATOM 1003 HE1 TYR A 71155.435 7.761 -1.254 1.00 0.00 H ATOM 1004 HE2 TYR A 71156.080 11.563 0.571 1.00 0.00 H ATOM 1005 HH TYR A 71156.854 9.955 -2.056 1.00 0.00 H ATOM 1006 N PHE A 72155.900 6.714 6.244 1.00 0.00 N ATOM 1007 CA PHE A 72155.480 6.283 7.572 1.00 0.00 C ATOM 1008 C PHE A 72156.457 5.262 8.147 1.00 0.00 C

ATOM 1009 O PHE A 72157.463 4.930 7.521 1.00 0.00 O ATOM 1010 CB PHE A 72154.074 5.683 7.515 1.00 0.00 C ATOM 1011 CG PHE A 72153.907 4.646 6.442 1.00 0.00 C ATOM 1012 CD1 PHE A 72153.991 3.296 6.745 1.00 0.00 C ATOM 1013 CD2 PHE A 72153.664 5.020 5.130 1.00 0.00 C ATOM 1014 CE1 PHE A 72153.838 2.340 5.760 1.00 0.00 C ATOM 1015 CE2 PHE A 72153.510 4.068 4.140 1.00 0.00 C ATOM 1016 CZ PHE A 72153.597 2.726 4.456 1.00 0.00 C ATOM 1017 H PHE A 72156.362 6.078 5.659 1.00 0.00 H ATOM 1018 HA PHE A 72155.466 7.150 8.214 1.00 0.00 H ATOM 1019 1HB PHE A 72153.850 5.219 8.463 1.00 0.00 H ATOM 1020 2HB PHE A 72153.361 6.474 7.328 1.00 0.00 H ATOM 1021 HD1 PHE A 72154.180 2.993 7.765 1.00 0.00 H ATOM 1022 HD2 PHE A 72153.597 6.069 4.882 1.00 0.00 H ATOM 1023 HE1 PHE A 72153.906 1.291 6.009 1.00 0.00 H ATOM 1024 HE2 PHE A 72153.321 4.372 3.121 1.00 0.00 H ATOM 1025 HZ PHE A 72153.476 1.980 3.684 1.00 0.00 H ATOM 1026 N THR A 73156.152 4.768 9.342 1.00 0.00 N ATOM 1027 CA THR A 73157.003 3.784 10.003 1.00 0.00 C ATOM 1028 C THR A 73156.260 2.467 10.201 1.00 0.00 C ATOM 1029 O THR A 73155.275 2.404 10.938 1.00 0.00 O ATOM 1030 CB THR A 73157.485 4.319 11.352 1.00 0.00 C ATOM 1031 OG1 THR A 73157.819 5.693 11.256 1.00 0.00 O ATOM 1032 CG2 THR A 73158.697 3.588 11.888 1.00 0.00 C ATOM 1033 H THR A 73155.336 5.071 9.791 1.00 0.00 H ATOM 1034 HA THR A 73157.860 3.608 9.369 1.00 0.00 H ATOM 1035 HB THR A 73156.689 4.214 12.075 1.00 0.00 H ATOM 1036 HG1 THR A 73157.943 6.054 12.137 1.00 0.00 H ATOM 1037 1HG2 THR A 73158.608 3.479 12.959 1.00 0.00 H ATOM 1038 2HG2 THR A 73159.589 4.151 11.656 1.00 0.00 H ATOM 1039 3HG2 THR A 73158.759 2.610 11.431 1.00 0.00 H ATOM 1040 N CYS A 74156.736 1.418 9.539 1.00 0.00 N ATOM 1041 CA CYS A 74156.116 0.102 9.643 1.00 0.00 C ATOM 1042 C CYS A 74157.174 -0.992 9.725 1.00 0.00 C ATOM 1043 O CYS A 74158.373 -0.717 9.671 1.00 0.00 O ATOM 1044 CB CYS A 74155.198 -0.148 8.444 1.00 0.00 C ATOM 1045 SG CYS A 74153.512 0.467 8.665 1.00 0.00 S ATOM 1046 H CYS A 74157.524 1.531 8.967 1.00 0.00 H ATOM 1047 HA CYS A 74155.525 0.085 10.546 1.00 0.00 H ATOM 1048 1HB CYS A 74155.613 0.339 7.575 1.00 0.00 H ATOM 1049 2HB CYS A 74155.140 -1.211 8.261 1.00 0.00 H ATOM 1050 HG CYS A 74153.269 0.955 7.875 1.00 0.00 H ATOM 1051 N ALAA 75156.723 -2.236 9.856 1.00 0.00 N ATOM 1052 CA ALAA 75157.631 -3.373 9.946 1.00 0.00 C ATOM 1053 C ALAA 75158.416 -3.552 8.652 1.00 0.00 C ATOM 1054 O ALAA 75158.263 -2.776 7.708 1.00 0.00 O ATOM 1055 CB ALAA 75156.857 -4.640 10.276 1.00 0.00 C ATOM 1056 H ALAA 75155.756 -2.393 9.894 1.00 0.00 H ATOM 1057 HA ALAA 75158.325 -3.183 10.752 1.00 0.00 H ATOM 1058 1HB ALA A 75156.841 -4.784 11.347 1.00 0.00 H ATOM 1059 2HB ALA A 75157.337 -5.487 9.807 1.00 0.00 H ATOM 1060 3HB ALA A 75155.846 -4.551 9.910 1.00 0.00 H ATOM 1061 N LEUA 76159.258 -4.580 8.613 1.00 0.00 N ATOM 1062 CA LEU A 76160.068 -4.861 7.434 1.00 0.00 C ATOM 1063 C LEUA 76159.357 -5.842 6.507 1.00 0.00 C ATOM 1064 O LEUA 76158.756 -6.816 6.960 1.00 0.00 O ATOM 1065 CB LEU A 76161.428 -5.427 7.847 1.00 0.00 C ATOM 1066 CG LEU A 76162.316 -4.465 8.637 1.00 0.00 C ATOM 1067 CD1 LEU A 76163.393 -5.228 9.391 1.00 0.00 C ATOM 1068 CD2 LEU A 76162.943 -3.436 7.708 1.00 0.00 C ATOM 1069 H LEUA 76159.336 -5.163 9.397 1.00 0.00 H ATOM 1070 HA LEU A 76160.219 -3.931 6.908 1.00 0.00 H

ATOM 1071 1HB LEU A 76161.259 -6.307 8.451 1.00 0.00 H ATOM 1072 2HB LEU A 76161.959 -5.720 6.954 1.00 0.00 H ATOM 1073 HG LEU A 76161.711 -3.938 9.361 1.00 0.00 H ATOM 1074 1HD1 LEU A 76164.253 -4.593 9.534 1.00 0.00 H ATOM 1075 2HD1 LEU A 76163.679 -6.102 8.824 1.00 0.00 H ATOM 1076 3HD1 LEU A 76163.009 -5.535 10.354 1.00 0.00 H ATOM 1077 1HD2 LEU A 76163.039 -3.855 6.717 1.00 0.00 H ATOM 1078 2HD2 LEU A 76163.920 -3.162 8.079 1.00 0.00 H ATOM 1079 3HD2 LEU A 76162.315 -2.558 7.666 1.00 0.00 H ATOM 1080 N LYS A 77159.429 -5.577 5.207 1.00 0.00 N ATOM 1081 CA LYS A 77158.793 -6.436 4.214 1.00 0.00 C ATOM 1082 C LYS A 77157.283 -6.478 4.419 1.00 0.00 C ATOM 1083 O LYS A 77156.656 -7.529 4.285 1.00 0.00 O ATOM 1084 CB LYS A 77159.370 -7.851 4.288 1.00 0.00 C ATOM 1085 CG LYS A 77160.884 -7.899 4.152 1.00 0.00 C ATOM 1086 CD LYS A 77161.333 -7.461 2.766 1.00 0.00 C ATOM 1087 CE LYS A 77162.582 -6.598 2.832 1.00 0.00 C ATOM 1088 NZ LYS A 77162.254 -5.158 3.023 1.00 0.00 N ATOM 1089 H LYS A 77159.924 -4.785 4.906 1.00 0.00 H ATOM 1090 HA LYS A 77159.001 -6.024 3.238 1.00 0.00 H ATOM 1091 1HB LYS A 77159.103 -8.287 5.239 1.00 0.00 H ATOM 1092 2HB LYS A 77158.940 -8.445 3.496 1.00 0.00 H ATOM 1093 1HG LYS A 77161.323 -7.240 4.887 1.00 0.00 H ATOM 1094 2HG LYS A 77161,220 -8.910 4.327 1.00 0.00 H ATOM 1095 1HD LYS A 77161.545 -8.337 2.174 1.00 0.00 H ATOM 1096 2HD LYS A 77160.538 -6.894 2.304 1.00 0.00 H ATOM 1097 1HE LYS A 77163.191 -6.930 3.660 1.00 0.00 H ATOM 1098 2HE LYS A 77163.134 -6.714 1.912 1.00 0.00 H ATOM 1099 1HZ LYS A 77161.291 -4.963 2.679 1.00 0.00 H ATOM 1100 2HZ LYS A 77162.925 -4.564 2.495 1.00 0.00 H ATOM 1101 3HZ LYS A 77162.307 -4.909 4.032 1.00 0.00 H

ATOM 1102 N LYS A 78156.702 -5.327 4.745 1.00 0.00 N ATOM 1103 CA LYS A 78155.265 -5.233 4.968 1.00 0.00 C ATOM 1104 C LYS A 78154.741 -3.857 4.567 1.00 0.00 C ATOM 1105 O LYS A 78153.838 -3.316 5.206 1.00 0.00 O ATOM 1106 CB LYS A 78154.936 -5.509 6.436 1.00 0.00 C ATOM 1107 CG LYS A 78155.439 -6.856 6.930 1.00 0.00 C ATOM 1108 CD LYS A 78155.044 -7.103 8.377 1.00 0.00 C ATOM 1109 CE LYS A 78153.565 -7.429 8.503 1.00 0.00 C ATOM 1110 NZ LYS A 78153.262 -8.159 9.765 1.00 0.00 N ATOM 1111 H LYS A 78157,254 -4.523 4.837 1.00 0.00 H ATOM 1112 HA LYS A 78154.785 -5.980 4.355 1.00 0.00 H ATOM 1113 1HB LYS A 78155.384 -4.737 7.045 1.00 0.00 H ATOM 1114 2HB LYS A 78153.864 -5.480 6.566 1.00 0.00 H ATOM 1115 1HG LYS A 78155.015 -7.635 6.314 1.00 0.00 H ATOM 1116 2HG LYS A 78156.516 -6.878 6.851 1.00 0.00 H ATOM 1117 1HD LYS A 78155.619 -7.932 8.760 1.00 0.00 H ATOM 1118 2HD LYS A 78155.259 -6.215 8.954 1.00 0.00 H ATOM 1119 1HE LYS A 78153.003 -6.507 8.487 1.00 0.00 H ATOM 1120 2HE LYS A 78153.271 -8.042 7.663 1.00 0.00 H ATOM 1121 1HZ LYS A 78153.299 -9.186 9.602 1.00 0.00 H ATOM 1122 2HZ LYS A 78152.312 -7.907 10.105 1.00 0.00 H ATOM 1123 3HZ LYS A 78153.957 -7.909 10.497 1.00 0.00 H ATOM 1124 N ALAA 79155.313 -3.298 3.507 1.00 0.00 N ATOM 1125 CA ALA A 79154.904 -1.986 3.022 1.00 0.00 C ATOM 1126 C ALA A 79154.827 -1.964 1.499 1.00 0.00 C ATOM 1127 O ALA A 79155.846 -1.846 0.817 1.00 0.00 O ATOM 1128 CB ALA A 79155.864 -0.916 3.519 1.00 0.00 C ATOM 1129 H ALA A 79156.028 -3.779 3.040 1.00 0.00 H ATOM 1130 HA ALA A 79153.924 -1.772 3.425 1.00 0.00 H ATOM 1131 1HB ALAA 79156.388 -1.279 4.391 1.00 0.00 H ATOM 1132 2HB ALA A 79155.310 -0.026 3.776 1.00 0.00 H ATOM 1133 3HB ALAA 79156.578 -0.684 2.741 1.00 0.00 H ATOM 1134 N LEU A 80153.612 -2.077 0.970 1.00 0.00 N ATOM 1135 CA LEU A 80153,402 -2.069 -0.473 1.00 0.00 C ATOM 1136 C LEU A 80152.484 -0.924 -0.884 1.00 0.00 C ATOM 1137 O LEUA 80151.354 -0.818 -0.407 1.00 0.00 O ATOM 1138 CB LEU A 80152.808 -3.404 -0.928 1.00 0.00 C ATOM 1139 CG LEU A 80152.489 -3.494 -2.422 1.00 0.00 C ATOM 1140 CD1 LEU A 80153.744 -3.825 -3.216 1.00 0.00 C ATOM 1141 CD2 LEU A 80151.407 -4.534 -2.673 1.00 0.00 C ATOM 1142 H LEUA 80152.839 -2.167 1.566 1.00 0.00 H ATOM 1143 HA LEU A 80154.362 -1.934 -0.947 1.00 0.00 H ATOM 1144 1HB LEU A 80153.508 -4.189 -0.682 1.00 0.00 H ATOM 1145 2HB LEU A 80151.894 -3.573 -0.378 1.00 0.00 H ATOM 1146 HG LEU A 80152.122 -2.537 -2.764 1.00 0.00 H ATOM 1147 1HD1 LEU A 80153.968 -4.877 -3.113 1.00 0.00 H ATOM 1148 2HD1 LEU A 80154.572 -3.243 -2.839 1.00 0.00 H ATOM 1149 3HD1 LEU A 80153.582 -3.590 -4.257 1.00 0.00 H ATOM 1150 1HD2 LEU A 80150.440 -4.054 -2.672 1.00 0.00 H ATOM 1151 2HD2 LEU A 80151.440 -5.282 -1.895 1.00 0.00 H ATOM 1152 3HD2 LEU A 80151.575 -5.003 -3.631 1.00 0.00 H ATOM 1153 N PHE A 81152.977 -0.065 -1.770 1.00 0.00 N ATOM 1154 CA PHE A 81152.201 1.074 -2.245 1.00 0.00 C ATOM 1155 C PHE A 81151.396 0.705 -3.487 1.00 0.00 C ATOM 1156 O PHE A 81151.813 -0.141 -4.280 1.00 0.00 O ATOM 1157 CB PHE A 81153.123 2.254 -2.554 1.00 0.00 C ATOM 1158 CG PHE A 81153.759 2.855 -1.332 1.00 0.00 C ATOM 1159 CD1 PHE A 81153.219 3.986 -0.740 1.00 0.00 C ATOM 1160 CD2 PHE A 81154.894 2.288 -0.775 1.00 0.00 C ATOM 1161 CE1 PHE A 81153.801 4.540 0.385 1.00 0.00 C ATOM 1162 CE2 PHE A 81155.479 2.838 0.349 1.00 0.00 C ATOM 1163 CZ PHE A 81154.932 3.966 0.930 1.00 0.00 C

ATOM 1164 H PHE A 81153.885 -0.201 -2.114 1.00 0.00 H ATOM 1165 HA PHE A 81151.517 1.359 -1.460 1.00 0.00 H ATOM 1166 1HB PHE A 81153.914 1.922 -3.209 1.00 0.00 H ATOM 1167 2HB PHE A 81152.554 3.027 -3.048 1.00 0.00 H ATOM 1168 HD1 PHE A 81152.335 4.436 -1.166 1.00 0.00 H ATOM 1169 HD2 PHE A 81155.323 1.406 -1.228 1.00 0.00 H ATOM 1170 HE1 PHE A 81153.371 5.423 0.835 1.00 0.00 H ATOM 1171 HE2 PHE A 81156.364 2.387 0.773 1.00 0.00 H ATOM 1172 HZ PHE A 81155.389 4.398 1.808 1.00 0.00 H ATOM 1173 N VALA 82150.242 1.343 -3.650 1.00 0.00 N ATOM 1174 CA VALA 82149.380 1.081 -4.796 1.00 0.00 C ATOM 1175 C VALA 82148.465 2.268 -5.077 1.00 0.00 C ATOM 1176 O VALA 82148.334 3.174 -4.253 1.00 0.00 O ATOM 1177 CB VALA 82148.517 -0.175 -4.574 1.00 0.00 C ATOM 1178 CG1 VAL A 82149.388 -1.419 -4.519 1.00 0.00 C ATOM 1179 CG2 VAL A 82147.691 -0.038 -3.304 1.00 0.00 C ATOM 1180 H VALA 82149.965 2.006 -2.984 1.00 0.00 H ATOM 1181 HA VALA 82150.010 0.912 -5.656 1.00 0.00 H ATOM 1182 HB VALA 82147.839 -0.273 -5.409 1.00 0.00 H ATOM 1183 1HG1 VAL A 82150.172 -1.344 -5.260 1.00 0.00 H ATOM 1184 2HG1 VAL A 82148.784 -2.291 -4.723 1.00 0.00 H ATOM 1185 3HG1 VAL A 82149.829 -1.508 -3.538 1.00 0.00 H ATOM 1186 1HG2 VAL A 82146.737 -0.526 -3.441 1.00 0.00 H ATOM 1187 2HG2 VAL A 82147.531 1.009 -3.090 1.00 0.00 H ATOM 1188 3HG2 VAL A 82148.217 -0.497 -2.480 1.00 0.00 H ATOM 1189 N LYS A 83147.834 2.257 -6.247 1.00 0.00 N ATOM 1190 CA LYS A 83146.931 3.333 -6.639 1.00 0.00 C ATOM 1191 C LYS A 83145.672 3.327 -5.778 1.00 0.00 C ATOM 1192 O LYS A 83144.950 2.332 -5.724 1.00 0.00 O ATOM 1193 CB LYS A 83146.554 3.198 -8.116 1.00 0.00 C ATOM 1194 CG LYS A 83147.716 3.442 -9.064 1.00 0.00 C

ATOM 1195 CD LYS A 83147.351 3.082 -10.495 1.00 0.00 C ATOM 1196 CE LYS A 83147.951 4.066-11.487 1.00 0.00 C ATOM 1197 NZ LYS A 83148.395 3.393 -12.739 1.00 0.00 N ATOM 1198 H LYS A 83147.979 1.508 -6.862 1.00 0.00 H ATOM 1199 HA LYS A 83147.446 4.270 -6.492 1.00 0.00 H ATOM 1200 1HB LYS A 83146.178 2.201 -8.289 1.00 0.00 H ATOM 1201 2HB LYS A 83145.776 3.912 -8.343 1.00 0.00 H ATOM 1202 1HG LYS A 83147.988 4.486 -9.024 1.00 0.00 H ATOM 1203 2HG LYS A 83148.555 2.837 -8.753 1.00 0.00 H ATOM 1204 1HD LYS A 83147.725 2.094 -10.715 1.00 0.00 H ATOM 1205 2HD LYS A 83146.276 3.093 -10.596 1.00 0.00 H ATOM 1206 1HE LYS A 83147.206 4.809 -11.733 1.00 0.00 H ATOM 1207 2HE LYS A 83148.800 4.549 -11.027 1.00 0.00 H ATOM 1208 1HZ LYS A 83148.832 2.476 -12.515 1.00 0.00 H ATOM 1209 2HZ LYS A 83149.090 3.984 -13.235 1.00 0.00 H ATOM 1210 3HZ LYS A 83147.580 3.233 -13.366 1.00 0.00 H ATOM 1211 N LEUA 84145.417 4.445 -5.109 1.00 0.00 N ATOM 1212 CA LEU A 84144.246 4.573 -4.250 1.00 0.00 C ATOM 1213 C LEU A 84142.961 4.378 -5.049 1.00 0.00 C ATOM 1214 O LEU A 84141.971 3.858 -4.535 1.00 0.00 O ATOM 1215 CB LEU A 84144.237 5.944 -3.571 1.00 0.00 C ATOM 1216 CG LEU A 84142.996 6.246 -2.730 1.00 0.00 C ATOM 1217 CD1 LEU A 84143.069 5.526 -1.392 1.00 0.00 C ATOM 1218 CD2 LEU A 84142.846 7.745 -2.522 1.00 0.00 C ATOM 1219 H LEU A 84146.031 5.204 -5.195 1.00 0.00 H ATOM 1220 HA LEU A 84144.305 3.805 -3.493 1.00 0.00 H ATOM 1221 1HB LEU A 84145.105 6.008 -2.929 1.00 0.00 H ATOM 1222 2HB LEU A 84144.320 6.701 -4.335 1.00 0.00 H ATOM 1223 HG LEU A 84142.120 5.890 -3.253 1.00 0.00 H ATOM 1224 1HD1 LEU A 84143.969 5.817 -0.874 1.00 0.00 H ATOM 1225 2HD1 LEU A 84143.079 4.458 -1.559 1.00 0.00 H ATOM 1226 3HD1 LEU A 84142.208 5.788 -0.795 1.00 0.00 H ATOM 1227 1HD2 LEU A 84143.594 8.088 -1.824 1.00 0.00 H ATOM 1228 2HD2 LEU A 84141.862 7.959 -2.130 1.00 0.00 H ATOM 1229 3HD2 LEU A 84142.974 8.254 -3.466 1.00 0.00 H ATOM 1230 N LYS A 85142.985 4.799 -6.310 1.00 0.00 N ATOM 1231 CA LYS A 85141.821 4.669 -7.179 1.00 0.00 C ATOM 1232 C LYS A 85141.476 3.201 -7.415 1.00 0.00 C ATOM 1233 O LYS A 85140.323 2.860 -7.676 1.00 0.00 O ATOM 1234 CB LYS A 85142.078 5.366 -8.517 1.00 0.00 C ATOM 1235 CG LYS A 85143.400 4.979 -9.161 1.00 0.00 C ATOM 1236 CD LYS A 85144.399 6.124 -9.118 1.00 0.00 C ATOM 1237 CE LYS A 85144.251 7.037 -10.325 1.00 0.00 C ATOM 1238 NZ LYS A 85144.698 8.426 -10.028 1.00 0.00 N ATOM 1239 H LYS A 85143.802 5.205 -6.663 1.00 0.00 H ATOM 1240 HA LYS A 85140.987 5.149 -6.689 1.00 0.00 H ATOM 1241 1HB LYS A 85141.281 5.111 -9.201 1.00 0.00 H ATOM 1242 2HB LYS A 85142.077 6.434 -8.360 1.00 0.00 H ATOM 1243 1HG LYS A 85143.814 4.134 -8.631 1.00 0.00 H ATOM 1244 2HG LYS A 85143.222 4.706 -10.191 1.00 0.00 H ATOM 1245 1HD LYS A 85144.235 6.700 -8.221 1.00 0.00 H ATOM 1246 2HD LYS A 85145.399 5.715 -9.109 1.00 0.00 H ATOM 1247 1HE LYS A 85144.847 6.643 -11.134 1.00 0.00 H ATOM 1248 2HE LYS A 85143.212 7.057 -10.619 1.00 0.00 H ATOM 1249 1HZ LYS A 85144.700 8.995 -10.899 1.00 0.00 H ATOM 1250 2HZ LYS A 85145.659 8.416 -9.632 1.00 0.00 H ATOM 1251 3HZ LYS A 85144.056 8.868 -9.338 1.00 0.00 H ATOM 1252 N SER A 86142.483 2.338 -7.322 1.00 0.00 N ATOM 1253 CA SER A 86142.283 0.908 -7.525 1.00 0.00 C ATOM 1254 C SER A 86142.180 0.177 -6.191 1.00 0.00 C ATOM 1255 O SER A 86142.582 -0.981 -6.073 1.00 0.00 O ATOM 1256 CB SER A 86143.430 0.324 -8.352 1.00 0.00 C

ATOM 1257 OG SER A 86143.578 1.016 -9.581 1.00 0.00 O ATOM 1258 H SER A 86143.380 2.669 -7.111 1.00 0.00 H ATOM 1259 HA SER A 86141.358 0.777 -8.067 1.00 0.00 H ATOM 1260 1HB SER A 86144.351 0.407 -7.794 1.00 0.00 H ATOM 1261 2HB SER A 86143.228 -0.716 -8.561 1.00 0.00 H ATOM 1262 HG SER A 86142.715 1.148 -9.979 1.00 0.00 H ATOM 1263 N CYS A 87141.639 0.860 -5.188 1.00 0.00 N ATOM 1264 CA CYS A 87141.482 0.275 -3.861 1.00 0.00 C ATOM 1265 C CYS A 87140.008 0.152 -3.491 1.00 0.00 C ATOM 1266 O CYS A 87139.153 0.819 -4.073 1.00 0.00 O ATOM 1267 CB CYS A 87142.211 1.124 -2.818 1.00 0.00 C ATOM 1268 SG CYS A 87143.995 0.839 -2.751 1.00 0.00 S ATOM 1269 H CYS A 87141.337 1.779 -5.343 1.00 0.00 H ATOM 1270 HA CYS A 87141.920 -0.712 -3.878 1.00 0.00 H ATOM 1271 1HB CYS A 87142.055 2.168 -3.041 1.00 0.00 H ATOM 1272 2HB CYS A 87141.806 0.906 -1.840 1.00 0.00 H ATOM 1273 HG CYS A 87144.366 1.082 -3.603 1.00 0.00 H ATOM 1274 N ARG A 88139.715 -0.707 -2.519 1.00 0.00 N ATOM 1275 CA ARG A 88138.344 -0.918 -2.072 1.00 0.00 C ATOM 1276 C ARG A 88138.274 -0.998 -0.547 1.00 0.00 C ATOM 1277 O ARG A 88139.152 -1.577 0.091 1.00 0.00 O ATOM 1278 CB ARG A 88137.777 -2.198 -2.689 1.00 0.00 C ATOM 1279 CG ARG A 88136.918 -1.952 -3.918 1.00 0.00 C ATOM 1280 CD ARG A 88135.437 -1.957 -3.574 1.00 0.00 C ATOM 1281 NE ARG A 88134.598 -2.033 -4.768 1.00 0.00 N ATOM 1282 CZ ARG A 88133.279 -2.220 -4.736 1.00 0.00 C ATOM 1283 NH1 ARG A 88132.649 -2.351 -3.576 1.00 0.00 N ATOM 1284 NH2 ARG A 88132.592 -2.276 -5.868 1.00 0.00 N ATOM 1285 H ARG A 88140.440 -1.210 -2.093 1.00 0.00 H ATOM 1286 HA ARG A 88137.756 -0.077 -2.406 1.00 0.00 H ATOM 1287 1HB ARG A 88138.597 -2.841 -2.972 1.00 0.00 H ATOM 1288 2HB ARG A 88137.173 -2.705 -1.950 1.00 0.00 H ATOM 1289 1HG ARG A 88137.176 -0.992 -4.340 1.00 0.00 H ATOM 1290 2HG ARG A 88137.113 -2.730 -4.642 1.00 0.00 H ATOM 1291 1HD ARG A 88135.230 -2.810 -2.946 1.00 0.00 H ATOM 1292 2HD ARG A 88135.203 -1.050 -3.037 1.00 0.00 H ATOM 1293 HE ARG A 88135.038 -1.938 -5.638 1.00 0.00 H ATOM 1294 1HH1 ARG A 88133.161 -2.310 -2.719 1.00 0.00 H ATOM 1295 2HH1 ARG A 88131.658 -2.491 -3.559 1.00 0.00 H ATOM 1296 1HH2 ARG A 88133.062 -2.176 -6.745 1.00 0.00 H ATOM 1297 2HH2 ARG A 88131.601 -2.416 -5.845 1.00 0.00 H ATOM 1298 N PRO A 89137.224 -0.415 0.060 1.00 0.00 N ATOM 1299 CA PRO A 89137.049 -0.428 1.516 1.00 0.00 C ATOM 1300 C PRO A 89137.081 -1.842 2.089 1.00 0.00 C ATOM 1301 O PRO A 89136.463 -2.756 1.545 1.00 0.00 O ATOM 1302 CB PRO A 89135.666 0.197 1.720 1.00 0.00 C ATOM 1303 CG PRO A 89135.435 1.020 0.501 1.00 0.00 C ATOM 1304 CD PRO A 89136.128 0.299 -0.621 1.00 0.00 C ATOM 1305 HA PRO A 89137.797 0.175 2.009 1.00 0.00 H ATOM 1306 1HB PRO A 89134.926 -0.584 1.817 1.00 0.00 H ATOM 1307 2HB PRO A 89135.672 0.807 2.612 1.00 0.00 H ATOM 1308 1HG PRO A 89134.376 1.093 0.303 1.00 0.00 H ATOM 1309 2HG PRO A 89135.862 2.003 0.634 1.00 0.00 H ATOM 1310 1HD PRO A 89135.452 -0.396 -1.098 1.00 0.00 H ATOM 1311 2HD PRO A 89136.516 1.005 -1.340 1.00 0.00 H ATOM 1312 N ASPA 90137.806 -2.014 3.189 1.00 0.00 N ATOM 1313 CA ASP A 90137.917 -3.316 3.835 1.00 0.00 C ATOM 1314 C ASPA 90136.972 -3.412 5.029 1.00 0.00 C ATOM 1315 O ASPA 90137.077 -2.637 5.980 1.00 0.00 O ATOM 1316 CB ASP A 90139.356 -3.565 4.287 1.00 0.00 C ATOM 1317 CG ASPA 90139.717 -5.038 4.282 1.00 0.00 C ATOM 1318 OD1 ASP A 90140.547 -5.448 5.120 1.00 0.00 O

ATOM 1319 OD2 ASP A 90139.169 -5.780 3.441 1.00 0.00 O ATOM 1320 H ASPA 90138.276 -1.246 3.577 1.00 0.00 H ATOM 1321 HA ASP A 90137.640 -4.068 3.111 1.00 0.00 H ATOM 1322 1HB ASP A 90140.030 -3.047 3.622 1.00 0.00 H ATOM 1323 2HB ASP A 90139.482 -3.185 5.290 1.00 0.00 H ATOM 1324 N SER A 91136.050 -4.367 4.972 1.00 0.00 N ATOM 1325 CA SER A 91135.087 -4.563 6.049 1.00 0.00 C ATOM 1326 C SER A 91135.527 -5.694 6.974 1.00 0.00 C ATOM 1327 O SER A 91134.698 -6.422 7.519 1.00 0.00 O ATOM 1328 CB SER A 91133.703 -4.870 5.475 1.00 0.00 C ATOM 1329 OG SER A 91132.679 -4.405 6.337 1.00 0.00 O ATOM 1330 H SER A 91136.017 -4.954 4.188 1.00 0.00 H ATOM 1331 HA SER A 91135.037 -3.649 6.618 1.00 0.00 H ATOM 1332 1HB SER A 91133.597 -4.383 4.517 1.00 0.00 H ATOM 1333 2HB SER A 91133.595 -5.937 5.350 1.00 0.00 H ATOM 1334 HG SER A 91131.982 -5.063 6.390 1.00 0.00 H ATOM 1335 N ARG A 92136.837 -5.835 7.146 1.00 0.00 N ATOM 1336 CA ARG A 92137.387 -6.876 8.006 1.00 0.00 C ATOM 1337 C ARG A 92137.020 -6.628 9.465 1.00 0.00 C ATOM 1338 O ARG A 92136.878 -7.568 10.247 1.00 0.00 O ATOM 1339 CB ARG A 92138.909 -6.940 7.854 1.00 0.00 C ATOM 1340 CG ARG A 92139.365 -7.676 6.605 1.00 0.00 C ATOM 1341 CD ARG A 92139.163 -9.177 6.737 1.00 0.00 C ATOM 1342 NE ARG A 92137.960 -9.631 6.042 1.00 0.00 N ATOM 1343 CZ ARG A 92137.717 -10.903 5.736 1.00 0.00 C ATOM 1344 NH1 ARG A 92138.590 -11.850 6.059 1.00 0.00 N ATOM 1345 NH2 ARG A 92136.599 -11.230 5.103 1.00 0.00 N ATOM 1346 H ARG A 92137.449 -5.222 6.686 1.00 0.00 H ATOM 1347 HA ARG A 92136.964 -7.819 7.695 1.00 0.00 H ATOM 1348 1HB ARG A 92139.298 -5.934 7.815 1.00 0.00 H ATOM 1349 2HB ARG A 92139.324 -7.444 8.715 1.00 0.00 H

ATOM 1350 1HG ARG A 92138.794 -7.320 5.761 1.00 0.00 H ATOM 1351 2HG ARG A 92140.414 -7.475 6.444 1.00 0.00 H ATOM 1352 1HD ARG A 92140.021 -9.681 6.317 1.00 0.00 H ATOM 1353 2HD ARG A 92139.078 -9.426 7.785 1.00 0.00 H ATOM 1354 HE ARG A 92137.299 -8.953 5.792 1.00 0.00 H ATOM 1355 1HH1 ARG A 92139.436 -11.610 6.536 1.00 0.00 H ATOM 1356 2HH1 ARG A 92138.402 -12.804 5.826 1.00 0.00 H ATOM 1357 1HH2 ARG A 92135.937 -10.522 4.858 1.00 0.00 H ATOM 1358 2HH2 ARG A 92136.416 -12.187 4.873 1.00 0.00 H ATOM 1359 N PHE A 93136.868 -5.358 9.825 1.00 0.00 N ATOM 1360 CA PHE A 93136.517 -4.988 11.192 1.00 0.00 C ATOM 1361 C PHE A 93135.373 -3.979 11.206 1.00 0.00 C ATOM 1362 O PHE A 93135.331 -3.085 12.051 1.00 0.00 O ATOM 1363 CB PHE A 93137.733 -4.406 11.914 1.00 0.00 C ATOM 1364 CG PHE A 93138.849 -5.395 12.101 1.00 0.00 C ATOM 1365 CD1 PHE A 93139.524 -5.913 11.008 1.00 0.00 C ATOM 1366 CD2 PHE A 93139.223 -5.804 13.372 1.00 0.00 C ATOM 1367 CE1 PHE A 93140.552 -6.822 11.178 1.00 0.00 C ATOM 1368 CE2 PHE A 93140.248 -6.713 13.547 1.00 0.00 C ATOM 1369 CZ PHE A 93140.913 -7.223 12.449 1.00 0.00 C ATOM 1370 H PHE A 93136.994 -4.652 9.157 1.00 0.00 H ATOM 1371 HA PHE A 93136.199 -5.882 11.705 1.00 0.00 H ATOM 1372 1HB PHE A 93138.119 -3.576 11.342 1.00 0.00 H ATOM 1373 2HB PHE A 93137.431 -4.056 12.889 1.00 0.00 H ATOM 1374 HD1 PHE A 93139.242 -5.600 10.014 1.00 0.00 H ATOM 1375 HD2 PHE A 93138.702 -5.407 14.231 1.00 0.00 H ATOM 1376 HE1 PHE A 93141.070 -7.219 10.317 1.00 0.00 H ATOM 1377 HE2 PHE A 93140.529 -7.025 14.542 1.00 0.00 H ATOM 1378 HZ PHE A 93141.716 -7.934 12.584 1.00 0.00 H ATOM 1379 N ALA A 94134.446 -4.128 10.266 1.00 0.00 N ATOM 1380 CA ALA A 94133.302 -3.230 10.171 1.00 0.00 C

ATOM 1381 C ALA A 94132.101 -3.789 10.924 1.00 0.00 C ATOM 1382 O ALA A 94131.718 -4.944 10.733 1.00 0.00 O ATOM 1383 CB ALA A 94132.944 -2.982 8.713 1.00 0.00 C ATOM 1384 H ALAA 94134.534 -4.860 9.620 1.00 0.00 H ATOM 1385 HA ALAA 94133.583 -2.285 10.613 1.00 0.00 H ATOM 1386 1HB ALA A 94132.185 -3.686 8.404 1.00 0.00 H ATOM 1387 2HB ALA A 94133.824 -3.111 8.100 1.00 0.00 H ATOM 1388 3HB ALA A 94132.570 -1.976 8.600 1.00 0.00 H ATOM 1389 N SER A 95131.509 -2.964 11.783 1.00 0.00 N ATOM 1390 CA SER A 95130.351 -3.376 12.566 1.00 0.00 C ATOM 1391 C SER A 95129.056 -3.097 11.811 1.00 0.00 C ATOM 1392 O SER A 95128.835 -1.988 11.325 1.00 0.00 O ATOM 1393 CB SER A 95130.336 -2.652 13.913 1.00 0.00 C ATOM 1394 OG SER A 95130.569 -1.263 13.749 1.00 0.00 O ATOM 1395 H SER A 95131.861 -2.056 11.891 1.00 0.00 H ATOM 1396 HA SER A 95130.430 -4.438 12.740 1.00 0.00 H ATOM 1397 1HB SER A 95129.372 -2.788 14.382 1.00 0.00 H ATOM 1398 2HB SER A 95131.107 -3.062 14.548 1.00 0.00 H ATOM 1399 HG SER A 95129.901 -0.892 13.169 1.00 0.00 H ATOM 1400 N LEUA 96128.201 -4.111 11.717 1.00 0.00 N ATOM 1401 CA LEU A 96126.927 -3.976 11.022 1.00 0.00 C ATOM 1402 C LEUA 96125.985 -5.119 11.386 1.00 0.00 C ATOM 1403 O LEU A 96126.309 -6.290 11.190 1.00 0.00 O ATOM 1404 CB LEU A 96127.150 -3.939 9.507 1.00 0.00 C ATOM 1405 CG LEU A 96127.031 -2.553 8.870 1.00 0.00 C ATOM 1406 CD1 LEU A 96127.658 -2.548 7.484 1.00 0.00 C ATOM 1407 CD2 LEU A 96125.573 -2.123 8.800 1.00 0.00 C ATOM 1408 H LEU A 96128.433 -4.971 12.126 1.00 0.00 H ATOM 1409 HA LEU A 96126.478 -3.044 11.333 1.00 0.00 H ATOM 1410 1HB LEU A 96128.137 -4.324 9.301 1.00 0.00 H ATOM 1411 2HB LEU A 96126.424 -4.588 9.040 1.00 0.00 H

ATOM 1412 HG LEU A 96127.563 -1.837 9.479 1.00 0.00 H ATOM 1413 1HD1 LEU A 96127.346 -3.430 6.944 1.00 0.00 H ATOM 1414 2HD1 LEU A 96128.733 -2.544 7.576 1.00 0.00 H ATOM 1415 3HD1 LEU A 96127.339 -1.666 6.948 1.00 0.00 H ATOM 1416 1HD2 LEU A 96124.961 -2.970 8.524 1.00 0.00 H ATOM 1417 2HD2 LEU A 96125.463 -1.344 8.060 1.00 0.00 H ATOM 1418 3HD2 LEU A 96125.261 -1.752 9.764 1.00 0.00 H ATOM 1419 N GLN A 97124.818 -4.770 11.919 1.00 0.00 N ATOM 1420 CA GLN A 97123.829 -5.767 12.312 1.00 0.00 C ATOM 1421 C GLN A 97122.418 -5.307 11.952 1.00 0.00 C ATOM 1422 O GLN A 97121.781 -4.580 12.715 1.00 0.00 O ATOM 1423 CB GLN A 97123.920 -6.040 13.814 1.00 0.00 C ATOM 1424 CG GLN A 97124.007 -4.778 14.657 1.00 0.00 C ATOM 1425 CD GLN A 97123.601 -5.011 16.100 1.00 0.00 C ATOM 1426 OE1 GLN A 97122.523 -4.598 16.527 1.00 0.00 O ATOM 1427 NE2 GLN A 97124.464 -5.675 16.858 1.00 0.00 N ATOM 1428 H GLN A 97124.618 -3.821 12.052 1.00 0.00 H ATOM 1429 HA GLN A 97124.047 -6.679 11.777 1.00 0.00 H ATOM 1430 1HB GLN A 97123.045 -6.593 14.122 1.00 0.00 H ATOM 1431 2HB GLN A 97124.798 -6.637 14.007 1.00 0.00 H ATOM 1432 1HG GLN A 97125.024 -4.418 14.640 1.00 0.00 H ATOM 1433 2HG GLN A 97123.354 -4.030 14.231 1.00 0.00 H ATOM 1434 1HE2 GLN A 97125.305 -5.974 16.450 1.00 0.00 H ATOM 1435 2HE2 GLN A 97124.228 -5.840 17.794 1.00 0.00 H ATOM 1436 N PRO A 98121.906 -5.725 10.780 1.00 0.00 N ATOM 1437 CA PRO A 98120.563 -5.349 10.327 1.00 0.00 C ATOM 1438 C PRO A 98119.501 -5.591 11.395 1.00 0.00 C ATOM 1439 O PRO A 98118.481 -4.905 11.436 1.00 0.00 O ATOM 1440 CB PRO A 98120.328 -6.262 9.121 1.00 0.00 C ATOM 1441 CG PRO A 98121.691 -6.560 8.604 1.00 0.00 C ATOM 1442 CD PRO A 98122.594 -6.595 9.805 1.00 0.00 C

ATOM 1443 HA PRO A 98120.526 -4.315 10.012 1.00 0.00 H ATOM 1444 1HB PRO A 98119.819 -7.160 9.441 1.00 0.00 H ATOM 1445 2HB PRO A 98119.730 -5.745 8.386 1.00 0.00 H ATOM 1446 1HG PRO A 98121.692 -7.519 8.105 1.00 0.00 H ATOM 1447 2HG PRO A 98122.004 -5.782 7.922 1.00 0.00 H ATOM 1448 1HD PRO A 98122.681 -7.602 10.184 1.00 0.00 H ATOM 1449 2HD PRO A 98123.568 -6.199 9.557 1.00 0.00 H ATOM 1450 N SER A 99119.751 -6.571 12.257 1.00 0.00 N ATOM 1451 CA SER A 99118.818 -6.903 13.328 1.00 0.00 C ATOM 1452 C SER A 99119.407 -6.553 14.690 1.00 0.00 C ATOM 1453 O SER A 99120.557 -6.884 14.983 1.00 0.00 O ATOM 1454 CB SER A 99118.462 -8.390 13.279 1.00 0.00 C ATOM 1455 OG SER A 99118.677 -8.924 11.984 1.00 0.00 O ATOM 1456 H SER A 99120.583 -7.081 12.174 1.00 0.00 H ATOM 1457 HA SER A 99117.920 -6.322 13.178 1.00 0.00 H ATOM 1458 1HB SER A 99119.079 -8.929 13.983 1.00 0.00 H ATOM 1459 2HB SER A 99117.422 -8.518 13.540 1.00 0.00 H ATOM 1460 HG SER A 99119.277 -9.671 12.041 1.00 0.00 H ATOM 1461 N GLY A 100118.614 -5.885 15.520 1.00 0.00 N ATOM 1462 CA GLY A 100119.076 -5.501 16.842 1.00 0.00 C ATOM 1463 C GLY A 100118.068 -5.831 17.927 1.00 0.00 C ATOM 1464 O GLY A 100116.862 -5.824 17.680 1.00 0.00 O ATOM 1465 H GLY A 100117.707 -5.647 15.233 1.00 0.00 H ATOM 1466 1HA GLY A 100119.999 -6.020 17.052 1.00 0.00 H ATOM 1467 2HA GLY A 100119.262 -4.437 16.850 1.00 0.00 H ATOM 1468 N PRO A 101118.536 -6.127 19.153 1.00 0.00 N ATOM 1469 CA PRO A 101117.654 -6.460 20.276 1.00 0.00 C ATOM 1470 C PRO A 101116.891 -5.245 20.792 1.00 0.00 C ATOM 1471 O PRO A 101117.052 -4.840 21.944 1.00 0.00 O ATOM 1472 CB PRO A 101118.620 -6.980 21.341 1.00 0.00 C ATOM 1473 CG PRO A 101119.916 -6.311 21.034 1.00 0.00 C

ATOM 1474 CD PRO A 101119.960 -6.160 19.538 1.00 0.00 C ATOM 1475 HA PRO A 101116.954 -7.238 20.010 1.00 0.00 H ATOM 1476 1HB PRO A 101118.258 -6.710 22.322 1.00 0.00 H ATOM 1477 2HB PRO A 101118.705 -8.054 21.263 1.00 0.00 H ATOM 1478 1HG PRO A 101119.950 -5.343 21.511 1.00 0.00 H ATOM 1479 2HG PRO A 101120.736 -6.926 21.373 1.00 0.00 H ATOM 1480 1HD PRO A 101120.453 -5.238 19.267 1.00 0.00 H ATOM 1481 2HD PRO A 101120.461 -7.003 19.088 1.00 0.00 H ATOM 1482 N SER A 102116.057 -4.667 19.933 1.00 0.00 N ATOM 1483 CA SER A 102115.268 -3.498 20.303 1.00 0.00 C ATOM 1484 C SER A 102113.913 -3.913 20.867 1.00 0.00 C ATOM 1485 O SER A 102113.606 -3.648 22.030 1.00 0.00 O ATOM 1486 CB SER A 102115.071 -2.585 19.091 1.00 0.00 C ATOM 1487 OG SER A 102114.531 -1.334 19.478 1.00 0.00 O ATOM 1488 H SER A 102115.971 -5.036 19.029 1.00 0.00 H ATOM 1489 HA SER A 102115.812 -2.959 21.064 1.00 0.00 H ATOM 1490 1HB SER A 102116.024 -2.418 18.611 1.00 0.00 H ATOM 1491 2HB SER A 102114.394 -3.057 18.394 1.00 0.00 H ATOM 1492 HG SER A 102115.179 -0.642 19.319 1.00 0.00 H ATOM 1493 N SER A 103113.105 -4.563 20.036 1.00 0.00 N ATOM 1494 CA SER A 103111.783 -5.015 20.452 1.00 0.00 C ATOM 1495 C SER A 103111.266 -6.112 19.527 1.00 0.00 C ATOM 1496 O SER A 103111.769 -6.290 18.418 1.00 0.00 O ATOM 1497 CB SER A 103110.802 -3.840 20.466 1.00 0.00 C ATOM 1498 OG SER A 103111.343 -2.733 21.164 1.00 0.00 O ATOM 1499 H SER A 103113.407 -4.745 19.121 1.00 0.00 H ATOM 1500 HA SER A 103111.868 -5.413 21.452 1.00 0.00 H ATOM 1501 1HB SER A 103110.587 -3.541 19.452 1.00 0.00 H ATOM 1502 2HB SER A 103109.887 -4.146 20.952 1.00 0.00 H ATOM 1503 HG SER A 103111.681 -3.022 22.014 1.00 0.00 H ATOM 1504 N GLY A 104110.261 -6.846 19.992 1.00 0.00 N

ATOM 1505 CA GLY A 104109.694 -7.916 19.194 1.00 0.00 C
ATOM 1506 C GLY A 104108.344 -8.374 19.712 1.00 0.00 C
ATOM 1507 O GLY A 104108.159 -9.597 19.890 1.00 0.00 O
ATOM 1508 OXT GLY A 104107.472 -7.510 19.941 1.00 0.00 O
ATOM 1509 H GLY A 104109.901 -6.658 20.885 1.00 0.00 H
ATOM 1510 1HA GLY A 104109.578 -7.571 18.178 1.00 0.00 H
ATOM 1511 2HA GLY A 104110.373 -8.756 19.203 1.00 0.00 H
TER 1512 GLY A 104

Three-Dimensional Structure Coordinate Table 6

ATOM 1 N GLY A 1112.318 9.750 -2.270 1.00 0.00 N ATOM 2 CA GLY A 1111.240 9.201 -3.139 1.00 0.00 C ATOM 3 C GLY A 1110.691 7.886 -2.623 1.00 0.00 C ATOM 4 O GLY A 1109.480 7.663 -2.635 1.00 0.00 O ATOM 5 1H GLY A 1113.178 9.172 -2.358 1.00 0.00 H ATOM 6 2H GLY A 1112.012 9.746 -1.276 1.00 0.00 H ATOM 7 3H GLY A 1112.539 10.727 -2.549 1.00 0.00 H ATOM 8 1HA GLY A 1110.435 9.918 -3.192 1.00 0.00 H ATOM 9 2HA GLY A 1111.637 9.047 -4.132 1.00 0.00 H ATOM10 N SER A 2111.584 7.013 -2.167 1.00 0.00 N ATOM11 CA SER A 2111.182 5.712 -1.643 1.00 0.00 C ATOM12 C SER A 2112.008 5.342 -0.415 1.00 0.00 C ATOM13 O SER A 2111.463 4.944 0.615 1.00 0.00 O ATOM14 CB SER A 2111.337 4.636 -2.718 1.00 0.00 C ATOM15 OG SER A 2110.409 4.831 -3.772 1.00 0.00 O ATOM16 H SER A 2112.534 7.249 -2.182 1.00 0.00 H ATOM17 HA SER A 2110.143 5.776 -1.357 1.00 0.00 H ATOM18 1HB SER A 2112.337 4.677 -3.125 1.00 0.00 H ATOM19 2HB SER A 2111.166 3.664 -2.280 1.00 0.00 H ATOM20 HG SER A 2109.545 5.031 -3.405 1.00 0.00 H

ATOM21 N SER A 3113.325 5.477 -0.531 1.00 0.00 N ATOM22 CA SER A 3114.226 5.157 0.571 1.00 0.00 C ATOM23 C SER A 3114.354 6.336 1.530 1.00 0.00 C ATOM24 O SER A 3114.036 6.223 2.713 1.00 0.00 O ATOM25 CB SER A 3115.604 4.770 0.033 1.00 0.00 C ATOM26 OG SER A 3116.188 5.838 -0.692 1.00 0.00 O ATOM27 H SER A 3113.700 5.799 -1.377 1.00 0.00 H ATOM28 HA SER A 3113.809 4.316 1.105 1.00 0.00 H ATOM29 1HB SER A 3116.252 4.515 0.859 1.00 0.00 H ATOM30 2HB SER A 3115.506 3.917 -0.623 1.00 0.00 H ATOM31 HG SER A 3117.117 5.913 -0.460 1.00 0.00 H ATOM32 N GLY A 4114.820 7.466 1.009 1.00 0.00 N ATOM33 CA GLY A 4114.983 8.649 1.833 1.00 0.00 C ATOM34 C GLYA 4116.174 8.550 2.765 1.00 0.00 C ATOM35 O GLY A 4116.069 8.004 3.863 1.00 0.00 O ATOM36 H GLYA 4115.058 7.497 0.060 1.00 0.00 H ATOM37 1HA GLY A 4115.113 9.507 1.190 1.00 0.00 H ATOM38 2HA GLY A 4114.089 8.787 2.424 1.00 0.00 H ATOM39 N SER A 5117.312 9.078 2.326 1.00 0.00 N ATOM40 CA SER A 5118.529 9.046 3.127 1.00 0.00 C ATOM41 C SER A 5119.241 10.395 3.092 1.00 0.00 C ATOM42 O SER A 5119.252 11.074 2.066 1.00 0.00 O ATOM43 CB SER A 5119.468 7.948 2.623 1.00 0.00 C ATOM44 OG SER A 5119.748 8.109 1.244 1.00 0.00 O ATOM45 H SER A 5117.334 9.500 1.441 1.00 0.00 H ATOM46 HA SER A 5118.249 8.827 4.147 1.00 0.00 H ATOM47 1HB SER A 5120.397 7.991 3.173 1.00 0.00 H ATOM48 2HB SER A 5119.006 6.984 2.774 1.00 0.00 H ATOM49 HG SER A 5120.660 7.865 1.070 1.00 0.00 H ATOM50 N SER A 6119.832 10.776 4.219 1.00 0.00 N ATOM51 CA SER A 6120.546 12.044 4.317 1.00 0.00 C

ATOM52 C SER A 6121.965 11.832 4.834 1.00 0.00 C ATOM53 O SER A 6122.531 12.701 5.498 1.00 0.00 O ATOM54 CB SER A 6119.794 13.006 5.238 1.00 0.00 C ATOM55 OG SER A 6118.457 13.187 4.805 1.00 0.00 O ATOM56 H SER A 6119.789 10.190 5.003 1.00 0.00 H ATOM57 HA SER A 6120.597 12.473 3.327 1.00 0.00 H ATOM58 1HB SER A 6119.782 12.606 6.240 1.00 0.00 H ATOM59 2HB SER A 6120.292 13.964 5.238 1.00 0.00 H ATOM60 HG SER A 6118.443 13.319 3.854 1.00 0.00 H ATOM61 N GLY A 7122.535 10.671 4.527 1.00 0.00 N ATOM62 CA GLY A 7123.883 10.367 4.969 1.00 0.00 C ATOM63 C GLY A 7124.017 8.950 5.488 1.00 0.00 C ATOM64 O GLY A 7123.400 8.587 6.490 1.00 0.00 O ATOM65 H GLY A 7122.036 10.016 3.995 1.00 0.00 H ATOM66 1HA GLY A 7124.561 10.500 4.139 1.00 0.00 H ATOM67 2HA GLY A 7124.155 11.054 5.756 1.00 0.00 H ATOM68 N LEU A 8124.825 8.144 4.805 1.00 0.00 N ATOM69 CA LEU A 8125.038 6.758 5.203 1.00 0.00 C ATOM70 C LEUA 8126.306 6.621 6.038 1.00 0.00 C ATOM71 O LEUA 8126.247 6.510 7.263 1.00 0.00 O ATOM72 CB LEU A 8125.123 5.858 3.969 1.00 0.00 C ATOM73 CG LEU A 8123.782 5.319 3.467 1.00 0.00 C ATOM74 CD1 LEU A 8123.953 4.629 2.123 1.00 0.00 C ATOM75 CD2 LEU A 8123.178 4.364 4.486 1.00 0.00 C ATOM76 H LEU A 8125.289 8.492 4.014 1.00 0.00 H ATOM77 HA LEU A 8124.196 6.453 5.801 1.00 0.00 H ATOM78 1HB LEU A 8125.583 6.421 3.169 1.00 0.00 H ATOM79 2HB LEU A 8125.757 5.017 4.205 1.00 0.00 H ATOM80 HG LEU A 8123.097 6.144 3.333 1.00 0.00 H ATOM81 1HD1 LEU A 8123.170 3.896 1.992 1.00 0.00 H ATOM82 2HD1 LEU A 8124.915 4.140 2.089 1.00 0.00 H ATOM83 3HD1 LEU A 8123.893 5.362 1.331 1.00 0.00 H ATOM84 1HD2 LEU A 8123.006 4.890 5.414 1.00 0.00 H ATOM85 2HD2 LEU A 8123.859 3.544 4.658 1.00 0.00 H ATOM86 3HD2 LEU A 8122.241 3.982 4.110 1.00 0.00 H ATOM87 N ALAA 9127.450 6.628 5.367 1.00 0.00 N ATOM88 CA ALA A 9128.735 6.505 6.044 1.00 0.00 C ATOM89 C ALAA 9129.891 6.773 5.085 1.00 0.00 C ATOM90 O ALAA 9130.601 5.854 4.679 1.00 0.00 O ATOM91 CB ALA A 9128.872 5.123 6.665 1.00 0.00 C ATOM92 H ALAA 9127.429 6.720 4.392 1.00 0.00 H ATOM93 HA ALA A 9128.764 7.235 6.839 1.00 0.00 H ATOM94 1HB ALA A 9127.891 4.724 6.876 1.00 0.00 H ATOM95 2HB ALA A 9129.436 5.195 7.583 1.00 0.00 H ATOM96 3HB ALA A 9129.387 4.468 5.978 1.00 0.00 H ATOM97 N MET A 10130.074 8.041 4.727 1.00 0.00 N ATOM98 CA MET A 10131.144 8.429 3.816 1.00 0.00 C ATOM99 C MET A 10131.191 9.946 3.646 1.00 0.00 C 100 O MET A 10130.954 10.465 2.554 1.00 0.00 O 101 CB MET A 10130.955 7.754 2.457 1.00 0.00 C ATOM 102 CG MET A 10129.539 7.863 1.913 1.00 0.00 C ATOM 103 SD MET A 10129.407 9.023 0.539 1.00 0.00 S **ATOM** 104 CE META 10129.163 7.897 -0.833 1.00 0.00 C **ATOM** 105 H MET A 10129.476 8.729 5.084 1.00 0.00 H **ATOM** 106 HA MET A 10132.078 8.099 4.245 1.00 0.00 H ATOM 107 1HB MET A 10131.628 8.210 1.746 1.00 0.00 H ATOM 108 2HB MET A 10131.202 6.707 2.551 1.00 0.00 H **ATOM** 109 1HG MET A 10129.223 6.888 1.573 1.00 0.00 H **ATOM** 110 2HG MET A 10128.887 8.193 2.709 1.00 0.00 H **ATOM** 111 1HE MET A 10130.124 7.587 -1.218 1.00 0.00 H **ATOM** 112 2HE MET A 10128.607 8.395 -1.613 1.00 0.00 H **ATOM** 113 3HE MET A 10128.615 7.031 -0.494 1.00 0.00 H ATOM

114 N PRO A 11131.502 10.682 4.727 1.00 0.00 N ATOM 115 CA PRO A 11131.579 12.145 4.688 1.00 0.00 C **ATOM** 116 C PRO A 11132.593 12.645 3.660 1.00 0.00 C **ATOM** 117 O PROA 11132.293 13.544 2.875 1.00 0.00 O ATOM 118 CB PRO A 11132.019 12.534 6.104 1.00 0.00 C **ATOM** 119 CG PRO A 11131.698 11.352 6.955 1.00 0.00 C **ATOM** 120 CD PRO A 11131.801 10.145 6.065 1.00 0.00 C **ATOM** 121 HA PRO A 11130.615 12.582 4.476 1.00 0.00 H **ATOM** 122 1HB PRO A 11133.076 12.749 6.109 1.00 0.00 H **ATOM** 123 2HB PRO A 11131.469 13.407 6.424 1.00 0.00 H **ATOM** 124 1HG PRO A 11132.411 11.280 7.761 1.00 0.00 H ATOM 125 2HG PRO A 11130.696 11.444 7.348 1.00 0.00 H **ATOM** 126 1HD PRO A 11132.798 9.733 6.102 1.00 0.00 H **ATOM** 127 2HD PRO A 11131.072 9.402 6.353 1.00 0.00 H ATOM 128 N PRO A 12133.809 12.066 3.642 1.00 0.00 N **ATOM** 129 CA PRO A 12134.853 12.465 2.692 1.00 0.00 C **ATOM** 130 C PROA 12134.377 12.375 1.247 1.00 0.00 C ATOM 131 O PRO A 12134.926 13.028 0.359 1.00 0.00 O **ATOM** 132 CB PRO A 12135.981 11.461 2.945 1.00 0.00 C **ATOM** 133 CG PRO A 12135.751 10.969 4.331 1.00 0.00 C **ATOM** 134 CD PRO A 12134.262 10.980 4.532 1.00 0.00 C ATOM 135 HA PRO A 12135.206 13.467 2.892 1.00 0.00 H ATOM 136 1HB PRO A 12135.918 10.658 2.225 1.00 0.00 H **ATOM** 137 2HB PRO A 12136.935 11.957 2.856 1.00 0.00 H **ATOM** 138 1HG PRO A 12136.135 9.965 4.434 1.00 0.00 H **ATOM** 139 2HG PRO A 12136.229 11.629 5.040 1.00 0.00 H **ATOM** 140 1HD PRO A 12133.834 10.034 4.236 1.00 0.00 H **ATOM** 141 2HD PRO A 12134.023 11.198 5.561 1.00 0.00 H ATOM 142 N GLY A 13133.351 11.559 1.017 1.00 0.00 N **ATOM** 143 CA GLY A 13132.818 11.397 -0.322 1.00 0.00 C ATOM 144 C GLY A 13133.068 10.012 -0.886 1.00 0.00 C **ATOM**

145 O GLY A 13132.330 9.545 -1.754 1.00 0.00 O ATOM **ATOM** 146 H GLY A 13132.954 11.064 1.765 1.00 0.00 H 147 1HA GLY A 13131.753 11.577 -0.298 1.00 0.00 H ATOM 148 2HA GLY A 13133.278 12.127 -0.972 1.00 0.00 H **ATOM** 149 N ASNA 14134.112 9.353 -0.393 1.00 0.00 N ATOM 150 CA ASN A 14134.459 8.014 -0.854 1.00 0.00 C **ATOM** 151 C ASN A 14133.299 7.045 -0.640 1.00 0.00 C ATOM 152 O ASNA 14132.195 7.453 -0.284 1.00 0.00 O **ATOM** 153 CB ASN A 14135.703 7.506 -0.122 1.00 0.00 C **ATOM** 154 CG ASN A 14136.823 8.529 -0.108 1.00 0.00 C **ATOM** 155 OD1 ASN A 14136.609 9.697 0.216 1.00 0.00 O **ATOM** 156 ND2 ASN A 14138.026 8.093 -0.460 1.00 0.00 N **ATOM** 157 H ASNA 14134.664 9.778 0.297 1.00 0.00 H **ATOM** 158 HA ASN A 14134.672 8.072 -1.911 1.00 0.00 H **ATOM** 159 1HB ASN A 14135.442 7.272 0.899 1.00 0.00 H **ATOM** 160 2HB ASN A 14136.062 6.613 -0.612 1.00 0.00 H **ATOM** 161 1HD2 ASN A 14138.123 7.149 -0.706 1.00 0.00 H **ATOM** 162 2HD2 ASN A 14138.769 8.733 -0.460 1.00 0.00 H **ATOM** 163 N SER A 15133.559 5.761 -0.861 1.00 0.00 N ATOM 164 CA SER A 15132.538 4.734 -0.693 1.00 0.00 C **ATOM** 165 C SER A 15132.234 4.506 0.785 1.00 0.00 C **ATOM** 166 O SER A 15131.163 4.867 1.271 1.00 0.00 O **ATOM** 167 CB SER A 15132.989 3.423 -1.341 1.00 0.00 C **ATOM** 168 OG SER A 15132.025 2.403 -1.154 1.00 0.00 O **ATOM** 169 H SER A 15134.460 5.496 -1.144 1.00 0.00 H **ATOM** 170 HA SER A 15131.639 5.077 -1.184 1.00 0.00 H **ATOM** 171 1HB SER A 15133.130 3.578 -2.400 1.00 0.00 H ATOM 172 2HB SER A 15133.921 3.108 -0.896 1.00 0.00 H **ATOM** 173 HG SER A 15132.121 2.027 -0.276 1.00 0.00 H ATOM 174 N HIS A 16133.184 3.902 1.492 1.00 0.00 N **ATOM**

175 CA HIS A 16133.019 3.626 2.914 1.00 0.00 C

ATOM

176 C HIS A 16133.864 4.578 3.754 1.00 0.00 C ATOM 177 O HIS A 16133.441 5.026 4.820 1.00 0.00 O **ATOM** 178 CB HIS A 16133.401 2.176 3.221 1.00 0.00 C ATOM 179 CG HIS A 16132.222 1.262 3.354 1.00 0.00 C **ATOM** 180 ND1 HIS A 16131.448 1.193 4.493 1.00 0.00 N **ATOM** 181 CD2 HIS A 16131.686 0.375 2.482 1.00 0.00 C **ATOM ATOM** 182 CE1 HIS A 16130.487 0.303 4.316 1.00 0.00 C 183 NE2 HIS A 16130.610 -0.207 3.104 1.00 0.00 N **ATOM** 184 H HIS A 16134.016 3.638 1.047 1.00 0.00 H **ATOM** 185 HA HIS A 16131.978 3.775 3.162 1.00 0.00 H ATOM 186 1HB HIS A 16134.024 1.800 2.424 1.00 0.00 H **ATOM ATOM** 187 2HB HIS A 16133.953 2.144 4.149 1.00 0.00 H 188 HD1 HIS A 16131.582 1.718 5.309 1.00 0.00 H **ATOM** 189 HD2 HIS A 16132.040 0.165 1.482 1.00 0.00 H **ATOM** 190 HE1 HIS A 16129.730 0.038 5.039 1.00 0.00 H **ATOM** 191 HE2 HIS A 16129.981 -0.833 2.688 1.00 0.00 H **ATOM** 192 N GLYA 17135.063 4.882 3.267 1.00 0.00 N **ATOM** 193 CA GLY A 17135.949 5.778 3.985 1.00 0.00 C **ATOM** 194 C GLYA 17137.401 5.349 3.901 1.00 0.00 C **ATOM** ATOM 195 O GLYA 17138.064 5.173 4.923 1.00 0.00 O 196 H GLYA 17135.348 4.495 2.413 1.00 0.00 H ATOM 197 1HA GLY A 17135.854 6.771 3.570 1.00 0.00 H **ATOM** 198 2HA GLY A 17135.654 5.805 5.024 1.00 0.00 H ATOM 199 N LEUA 18137.897 5.182 2.678 1.00 0.00 N **ATOM** 200 CA LEU A 18139.279 4.771 2.465 1.00 0.00 C **ATOM** 201 C LEUA 18140.246 5.872 2.888 1.00 0.00 C **ATOM** 202 O LEUA 18140.497 6.814 2.136 1.00 0.00 O **ATOM** 203 CB LEU A 18139.506 4.415 0.994 1.00 0.00 C **ATOM** 204 CG LEU A 18138.484 3.445 0.398 1.00 0.00 C **ATOM** 205 CD1 LEU A 18138.481 3.540 -1.120 1.00 0.00 C **ATOM** 206 CD2 LEU A 18138.781 2.021 0.844 1.00 0.00 C ATOM

207 H LEUA 18137.318 5.338 1.903 1.00 0.00 H ATOM 208 HA LEU A 18139.462 3.895 3.070 1.00 0.00 H 209 1HB LEU A 18139.484 5.328 0.417 1.00 0.00 H **ATOM** ATOM 210 2HB LEU A 18140.486 3.972 0.900 1.00 0.00 H 211 HG LEUA 18137.498 3.709 0.751 1.00 0.00 H ATOM 212 1HD1 LEU A 18138.860 4.506 -1.421 1.00 0.00 H ATOM 213 2HD1 LEU A 18137.472 3.419 -1.485 1.00 0.00 H ATOM 214 3HD1 LEU A 18139.109 2.763 -1.530 1.00 0.00 H ATOM 215 1HD2 LEU A 18139.591 1.619 0.254 1.00 0.00 H 216 2HD2 LEU A 18137.899 1.411 0.709 1.00 0.00 H ATOM 217 3HD2 LEU A 18139.061 2.021 1.887 1.00 0.00 H ATOM 218 N GLUA 19140.783 5.748 4.096 1.00 0.00 N ATOM 219 CA GLUA 19141.722 6.733 4.621 1.00 0.00 C **ATOM** 220 C GLUA 19142.809 6.061 5.452 1.00 0.00 C ATOM 221 O GLUA 19142.810 4.843 5.622 1.00 0.00 O ATOM 222 CB GLU A 19140.984 7.772 5.467 1.00 0.00 C ATOM 223 CG GLU A 19140.233 7.174 6.645 1.00 0.00 C 224 CD GLUA 19139.754 8.226 7.625 1.00 0.00 C ATOM 225 OE1 GLU A 19140.533 9.155 7.928 1.00 0.00 O **ATOM** 226 OE2 GLU A 19138.599 8:123 8.091 1.00 0.00 O **ATOM** 227 H GLUA 19140.544 4.976 4.650 1.00 0.00 H **ATOM** 228 HA GLUA 19142.184 7.230 3.779 1.00 0.00 H ATOM 229 1HB GLU A 19141.702 8.483 5.849 1.00 0.00 H **ATOM** ATOM 230 2HB GLU A 19140.274 8.291 4.841 1.00 0.00 H 231 1HG GLU A 19139.375 6.635 6.272 1.00 0.00 H ATOM 232 2HG GLU A 19140.888 6.490 7.164 1.00 0.00 H **ATOM** 233 N VALA 20143.732 6.865 5.969 1.00 0.00 N ATOM 234 CA VALA 20144.825 6.349 6.785 1.00 0.00 C ATOM ATOM 235 C VALA 20144.297 5.620 8.015 1.00 0.00 C 236 O VALA 20143.530 6.181 8.799 1.00 0.00 O ATOM ATOM 237 CB VALA 20145.770 7.479 7.235 1.00 0.00 C

238 CG1 VAL A 20146.993 6.908 7.939 1.00 0.00 C 239 CG2 VAL A 20146.181 8.337 6.049 1.00 0.00 C ATOM 240 H VALA 20143.678 7.829 5.798 1.00 0.00 H 241 HA VALA 20145.391 5.654 6.182 1.00 0.00 H **ATOM** ATOM 242 HB VALA 20145.240 8.105 7.938 1.00 0.00 H 243 1HG1 VAL A 20146.795 6.830 8.997 1.00 0.00 H **ATOM** 244 2HG1 VAL A 20147.838 7.559 7.777 1.00 0.00 H ATOM 245 3HG1 VAL A 20147.211 5.928 7.540 1.00 0.00 H ATOM 246 1HG2 VAL A 20145.398 9.046 5.828 1.00 0.00 H **ATOM** 247 2HG2 VAL A 20146.348 7.705 5.189 1.00 0.00 H ATOM 248 3HG2 VAL A 20147.091 8.868 6.287 1.00 0.00 H ATOM 249 N GLYA 21144.711 4.369 8.179 1.00 0.00 N ATOM 250 CA GLY A 21144.269 3.583 9.316 1.00 0.00 C **ATOM** 251 C GLYA 21143.228 2.548 8.939 1.00 0.00 C **ATOM** 252 O GLY A 21143.210 1.447 9.489 1.00 0.00 O ATOM 253 H GLY A 21145.322 3.975 7.522 1.00 0.00 H ATOM ATOM 254 1HA GLY A 21145.123 3.080 9.745 1.00 0.00 H 255 2HA GLY A 21143.847 4.248 10.056 1.00 0.00 H ATOM 256 N SER A 22142.359 2.901 7.997 1.00 0.00 N ATOM 257 CA SER A 22141.310 1.995 7.546 1.00 0.00 C ATOM 258 C SER A 22141.877 0.922 6.622 1.00 0.00 C ATOM 259 O SER A 22142.764 1.192 5.812 1.00 0.00 O **ATOM** 260 CB SER A 22140.208 2.774 6.826 1.00 0.00 C **ATOM** 261 OG SER A 22139.268 3.299 7.747 1.00 0.00 O **ATOM** 262 H SER A 22142.425 3.793 7.596 1.00 0.00 H ATOM 263 HA SER A 22140.889 1.516 8.417 1.00 0.00 H **ATOM** 264 1HB SER A 22140.649 3.592 6.276 1.00 0.00 H ATOM 265 2HB SER A 22139.694 2.116 6.141 1.00 0.00 H ATOM 266 HG SER A 22138.475 3.569 7.277 1.00 0.00 H ATOM 267 N LEUA 23141.359 -0.295 6.749 1.00 0.00 N **ATOM** 268 CA LEU A 23141.815 -1.410 5.924 1.00 0.00 C ATOM

269 C LEUA 23141.296 -1.278 4.496 1.00 0.00 C ATOM 270 O LEUA 23140.234 -0.702 4.261 1.00 0.00 O **ATOM** 271 CB LEU A 23141.353 -2.738 6.526 1.00 0.00 C 272 CG LEU A 23141.931 -3.059 7.905 1.00 0.00 C ATOM 273 CD1 LEU A 23140.954 -3.903 8.709 1.00 0.00 C **ATOM** 274 CD2 LEU A 23143.268 -3.773 7.769 1.00 0.00 C ATOM 275 H LEUA 23140.655 -0.449 7.412 1.00 0.00 H 276 HA LEU A 23142.894 -1.388 5.907 1.00 0.00 H ATOM 277 1HB LEU A 23140.276 -2.718 6.605 1.00 0.00 H **ATOM ATOM** 278 2HB LEU A 23141.633 -3.531 5.850 1.00 0.00 H 279 HG LEU A 23142.096 -2.137 8.443 1.00 0.00 H ATOM **ATOM** 280 1HD1 LEU A 23140.921 -4.902 8.302 1.00 0.00 H 281 2HD1 LEU A 23139.970 -3.460 8.659 1.00 0.00 H ATOM 282 3HD1 LEU A 23141.277 -3.944 9.739 1.00 0.00 H **ATOM** 283 1HD2 LEU A 23143.908 -3.500 8.594 1.00 0.00 H ATOM 284 2HD2 LEU A 23143.736 -3.485 6.840 1.00 0.00 H ATOM 285 3HD2 LEU A 23143.107 -4.841 7.776 1.00 0.00 H **ATOM** 286 N ALAA 24142.055 -1.814 3.546 1.00 0.00 N **ATOM** 287 CA ALAA 24141.672 -1.757 2.140 1.00 0.00 C ATOM 288 C ALAA 24142.245 -2.941 1.367 1.00 0.00 C **ATOM** 289 O ALAA 24143.206 -3.573 1.804 1.00 0.00 O **ATOM** 290 CB ALAA 24142.135 -0.447 1.520 1.00 0.00 C ATOM 291 H ALAA 24142.890 -2.260 3.795 1.00 0.00 H ATOM 292 HA ALA A 24140.593 -1.793 2.086 1.00 0.00 H ATOM 293 1HB ALA A 24143.026 -0.105 2.025 1.00 0.00 H ATOM 294 2HB ALA A 24141.356 0.295 1.623 1.00 0.00 H ATOM 295 3HB ALA A 24142.350 -0.601 0.473 1.00 0.00 H ATOM 296 N GLUA 25141.647 -3.236 0.217 1.00 0.00 N **ATOM** 297 CA GLU A 25142.098 -4.344 -0.617 1.00 0.00 C **ATOM** 298 C GLUA 25142.441 -3.863 -2.023 1.00 0.00 C ATOM ATOM 299 O GLU A 25141.810 -2.945 -2.547 1.00 0.00 O

- ATOM 300 CB GLU A 25141.023 -5.430 -0.684 1.00 0.00 C
- ATOM 301 CG GLU A 25141.523 -6.747 -1.252 1.00 0.00 C
- ATOM 302 CD GLUA 25140,399 -7.623 -1.770 1.00 0.00 C
- ATOM 303 OE1 GLU A 25140.407 -7.947 -2.976 1.00 0.00 O
- ATOM 304 OE2 GLU A 25139.511 -7.986 -0.970 1.00 0.00 O
- ATOM 305 H GLU A 25140.885 -2.695 -0.079 1.00 0.00 H
- ATOM 306 HA GLU A 25142.987 -4.758 -0.164 1.00 0.00 H
- ATOM 307 1HB GLU A 25140.646 -5.611 0.311 1.00 0.00 H
- ATOM 308 2HB GLU A 25140.212 -5.078 -1.306 1.00 0.00 H
- ATOM 309 1HG GLU A 25142.200 -6.540 -2.066 1.00 0.00 H
- ATOM 310 2HG GLU A 25142.048 -7.283 -0.475 1.00 0.00 H
- ATOM 311 N VALA 26143.445 -4.489 -2.629 1.00 0.00 N
- ATOM 312 CA VAL A 26143.872 -4.124 -3.974 1.00 0.00 C
- ATOM 313 C VALA 26143.444 -5.178 -4.990 1.00 0.00 C
- ATOM 314 O VALA 26143.415 -6.370 -4.688 1.00 0.00 O
- ATOM 315 CB VAL A 26145.399 -3.944 -4.051 1.00 0.00 C
- ATOM 316 CG1 VAL A 26145.804 -3.375 -5.401 1.00 0.00 C
- ATOM 317 CG2 VAL A 26145.890 -3.054 -2.919 1.00 0.00 C
- ATOM 318 H VALA 26143.910 -5.212 -2.160 1.00 0.00 H
- ATOM 319 HA VALA 26143.406 -3.183 -4.229 1.00 0.00 H
- ATOM 320 HB VAL A 26145.861 -4.915 -3.942 1.00 0.00 H
- ATOM 321 1HG1 VAL A 26146.882 -3.336 -5.467 1.00 0.00 H
- ATOM 322 2HG1 VAL A 26145.401 -2.378 -5.506 1.00 0.00 H
- ATOM 323 3HG1 VAL A 26145.418 -4.005 -6.188 1.00 0.00 H
- ATOM 324 1HG2 VAL A 26145.976 -3.637 -2.013 1.00 0.00 H
- ATOM 325 2HG2 VAL A 26145.186 -2.250 -2.763 1.00 0.00 H
- ATOM 326 3HG2 VAL A 26146.855 -2.643 -3.175 1.00 0.00 H
- ATOM 327 N LYS A 27143.116 -4.729 -6.197 1.00 0.00 N
- ATOM 328 CA LYS A 27142.690 -5.633 -7.259 1.00 0.00 C
- ATOM 329 C LYS A 27143.880 -6.082 -8.101 1.00 0.00 C
- ATOM 330 O LYS A 27144.102 -5.577 -9.201 1.00 0.00 O

331 CB LYS A 27141.647 -4.954 -8.149 1.00 0.00 C ATOM 332 CG LYS A 27140.301 -4.761 -7.470 1.00 0.00 C **ATOM** 333 CD LYS A 27139.285 -5.786 -7.945 1.00 0.00 C **ATOM ATOM** 334 CE LYS A 27139.368 -7.071 -7.135 1.00 0.00 C 335 NZ LYS A 27138.350 -7.109 -6.048 1.00 0.00 N ATOM 336 H LYS A 27143.160 -3.766 -6.378 1.00 0.00 H **ATOM** 337 HA LYS A 27142.245 -6.501 -6.796 1.00 0.00 H **ATOM** 338 1HB LYS A 27142.021 -3.983 -8.443 1.00 0.00 H **ATOM** 339 2HB LYS A 27141.499 -5.556 -9.034 1.00 0.00 H **ATOM** 340 1HG LYS A 27140.429 -4.864 -6.403 1.00 0.00 H **ATOM** 341 2HG LYS A 27139.933 -3.771 -7.698 1.00 0.00 H **ATOM** 342 1HD LYS A 27138.293 -5.372 -7.841 1.00 0.00 H **ATOM ATOM** 343 2HD LYS A 27139.475 -6.014 -8.984 1.00 0.00 H 344 1HE LYS A 27139.208 -7.909 -7.795 1.00 0.00 H ATOM 345 2HE LYS A 27140.353 -7.141 -6.697 1.00 0.00 H **ATOM** 346 1HZ LYS A 27137.554 -6.482 -6.282 1.00 0.00 H ATOM 347 2HZ LYS A 27138.772 -6.795 -5.152 1.00 0.00 H **ATOM** 348 3HZ LYS A 27137.992 -8.078 -5.928 1.00 0.00 H **ATOM** 349 N GLUA 28144.644 -7.034 -7.575 1.00 0.00 N **ATOM** 350 CA GLU A 28145.812 -7.553 -8.278 1.00 0.00 C **ATOM** 351 C GLUA 28145.714 -9.064 -8.456 1.00 0.00 C **ATOM** 352 O GLUA 28144.671 -9.664 -8.195 1.00 0.00 O **ATOM** 353 CB GLU A 28147.091 -7.198 -7.514 1.00 0.00 C ATOM 354 CG GLU A 28148.178 -6.601 -8.394 1.00 0.00 C ATOM 355 CD GLUA 28149.554 -7.148 -8.072 1.00 0.00 C **ATOM** 356 OE1 GLU A 28150.418 -7.154 -8.976 1.00 0.00 O **ATOM** 357 OE2 GLU A 28149.770 -7.572 -6.918 1.00 0.00 O **ATOM** 358 H GLU A 28144.417 -7.397 -6.694 1.00 0.00 H **ATOM** 359 HA GLU A 28145.846 -7.088 -9.252 1.00 0.00 H **ATOM** 360 1HB GLU A 28146.849 -6.482 -6.743 1.00 0.00 H **ATOM** 361 2HB GLU A 28147.483 -8.092 -7.052 1.00 0.00 H ATOM

- 362 1HG GLUA 28147.952 -6.824 -9.426 1.00 0.00 H ATOM
- 363 2HG GLUA 28148.190 -5.530 -8.252 1.00 0.00 H ATOM
- 364 N ASNA 29146.807 -9.675 -8.902 1.00 0.00.N ATOM
- 365 CA ASN A 29146.843 -11.117 -9.113 1.00 0.00 C ATOM
- 366 C ASN A 29146.916 -11.858 -7.781 1.00 0.00 C ATOM
- 367 O ASNA 29146.049 -12.673 -7.467 1.00 0.00 O ATOM
- 368 CB ASN A 29148.038 -11.495 -9.992 1.00 0.00 C ATOM
- 369 CG ASN A 29147.648 -11.689 -11.445 1.00 0.00 C ATOM
- 370 OD1 ASN A 29147.487 -12.817 -11.911 1.00 0.00 O **ATOM**
- 371 ND2 ASN A 29147.495 -10.586 -12.168 1.00 0.00 N ATOM
- 372 H ASN A 29147.608 -9.143 -9.092 1.00 0.00 H **ATOM**
- 373 HA ASN A 29145.932 -11.400 -9.619 1.00 0.00 H ATOM
- 374 1HB ASN A 29148.778 -10.711 -9.939 1.00 0.00 H **ATOM**
- 375 2HB ASN A 29148.468 -12.416 -9.627 1.00 0.00 H **ATOM**
- 376 1HD2 ASN A 29147.640 -9.721 -11.730 1.00 0.00 H ATOM
- 377 2HD2 ASN A 29147.244 -10.682 -13.110 1.00 0.00 H **ATOM**
- 378 N PRO A 30147.958 -11.585 -6.976 1.00 0.00 N ATOM
- 379 CA PRO A 30148.142 -12.228 -5.674 1.00 0.00 C **ATOM**
- 380 C PRO A 30147.254 -11.613 -4.593 1.00 0.00 C ATOM
- 381 O PRO A 30147.455 -10.466 -4.194 1.00 0.00 O ATOM
- 382 CB PRO A 30149.614 -11.962 -5.367 1.00 0.00 C ATOM
- 383 CG PRO A 30149.906 -10.665 -6.040 1.00 0.00 C **ATOM**
- 384 CD PRO A 30149.040 -10.624 -7.274 1.00 0.00 C ATOM
- 385 HA PRO A 30147.968 -13.291 -5.727 1.00 0.00 H **ATOM**
- 386 1HB PRO A 30149.757 -11.895 -4.298 1.00 0.00 H **ATOM**
- 387 2HB PRO A 30150.220 -12.760 -5.769 1.00 0.00 H **ATOM**
- 388 1HG PRO A 30149.657 -9.846 -5.381 1.00 0.00 H

ATOM

- 389 2HG PRO A 30150.949 -10.622 -6.315 1.00 0.00 H ATOM
- 390 1HD PRO A 30148.643 -9.631 -7.420 1.00 0.00 H ATOM
- 391 2HD PRO A 30149.604 -10.936 -8.140 1.00 0.00 H ATOM
- 392 N PRO A 31146.253 -12.366 -4.102 1.00 0.00 N

393 CA PRO A 31145.337 -11.880 -3.063 1.00 0.00 C 394 C PRO A 31146.064 -11.536 -1.768 1.00 0.00 C **ATOM** 395 O PRO A 31146.500 -12.422 -1.034 1.00 0.00 O **ATOM** 396 CB PRO A 31144.378 -13.056 -2.838 1.00 0.00 C **ATOM** 397 CG PRO A 31144.514 -13.909 -4.053 1.00 0.00 C **ATOM** 398 CD PRO A 31145.932 -13.743 -4.514 1.00 0.00 C **ATOM** 399 HA PRO A 31144.781 -11.018 -3.401 1.00 0.00 H **ATOM** 400 1HB PRO A 31144.666 -13.593 -1.946 1.00 0.00 H **ATOM** 401 2HB PRO A 31143.369 -12.685 -2.730 1.00 0.00 H **ATOM** 402 1HG PRO A 31144.319 -14.940 -3.802 1.00 0.00 H **ATOM** 403 2HG PRO A 31143.829 -13.571 -4.817 1.00 0.00 H **ATOM** 404 1HD PRO A 31146.576 -14.455 -4.020 1.00 0.00 H **ATOM** 405 2HD PRO A 31145.997 -13.849 -5.586 1.00 0.00 H **ATOM** 406 N PHE A 32146.191 -10.242 -1.492 1.00 0.00 N ATOM 407 CA PHE A 32146.864 -9.781 -0.283 1.00 0.00 C **ATOM ATOM** 408 C PHE A 32146.068 -8.670 0.395 1.00 0.00 C **ATOM** 409 O PHE A 32145.464 -7.831 -0.273 1.00 0.00 O 410 CB PHE A 32148.273 -9.285 -0.615 1.00 0.00 C ATOM 411 CG PHE A 32148.295 -8.133 -1.580 1.00 0.00 C 412 CD1 PHE A 32147.870 -6.875 -1.187 1.00 0.00 C ATOM 413 CD2 PHE A 32148.741 -8.311 -2.879 1.00 0.00 C ATOM ATOM 414 CE1 PHE A 32147.889 -5.815 -2.073 1.00 0.00 C 415 CE2 PHE A 32148.763 -7.254 -3.769 1.00 0.00 C ATOM 416 CZ PHE A 32148.337 -6.004 -3.366 1.00 0.00 C ATOM 417 H PHE A 32145.822 -9.581 -2.115 1.00 0.00 H ATOM 418 HA PHE A 32146.938 -10.618 0.394 1.00 0.00 H **ATOM** 419 1HB PHE A 32148.757 -8.964 0.295 1.00 0.00 H **ATOM** 420 2HB PHE A 32148.839 -10.095 -1.050 1.00 0.00 H ATOM 421 HD1 PHE A 32147.520 -6.724 -0.176 1.00 0.00 H ATOM 422 HD2 PHE A 32149.076 -9.288 -3.196 1.00 0.00 H **ATOM** ATOM 423 HE1 PHE A 32147.554 -4.838 -1.755 1.00 0.00 H

424 HE2 PHE A 32149.113 -7.405 -4.780 1.00 0.00 H 425 HZ PHE A 32148.352 -5.177 -4.059 1.00 0.00 H **ATOM** 426 N TYR A 33146.071 -8.673 1.724 1.00 0.00 N ATOM 427 CA TYR A 33145.349 -7.666 2.492 1.00 0.00 C 428 C TYR A 33146.315 -6.689 3.153 1.00 0.00 C ATOM 429 O TYR A 33147.406 -7.072 3.575 1.00 0.00 O ATOM 430 CB TYR A 33144.475 -8.335 3.555 1.00 0.00 C **ATOM** 431 CG TYR A 33143.212 -8.953 2.999 1.00 0.00 C **ATOM ATOM** 432 CD1 TYR A 33142.857 -10.258 3.318 1.00 0.00 C 433 CD2 TYR A 33142.375 -8.232 2.157 1.00 0.00 C **ATOM** 434 CE1 TYR A 33141.704 -10.828 2.811 1.00 0.00 C ATOM 435 CE2 TYR A 33141.220 -8.794 1.647 1.00 0.00 C **ATOM** 436 CZ TYR A 33140.888 -10.091 1.977 1.00 0.00 C ATOM 437 OH TYR A 33139.740 -10.655 1.473 1.00 0.00 O **ATOM** 438 H TYR A 33146.571 -9.369 2.199 1.00 0.00 H ATOM ATOM 439 HA TYR A 33144.715 -7.121 1.809 1.00 0.00 H **ATOM** 440 1HB TYR A 33145.042 -9.116 4.037 1.00 0.00 H 441 2HB TYR A 33144.188 -7.598 4.290 1.00 0.00 H ATOM 442 HD1 TYR A 33143.497 -10.832 3.971 1.00 0.00 H ATOM **ATOM** 443 HD2 TYR A 33142.637 -7.216 1.900 1.00 0.00 H **ATOM** 444 HE1 TYR A 33141.445 -11.844 3.070 1.00 0.00 H 445 HE2 TYR A 33140.581 -8.217 0.994 1.00 0.00 H **ATOM** 446 HH TYR A 33139.799 -10.701 0.515 1.00 0.00 H **ATOM** 447 N GLY A 34145.909 -5.427 3.237 1.00 0.00 N ATOM 448 CA GLY A 34146.751 -4.416 3.848 1.00 0.00 C **ATOM** 449 C GLY A 34145.959 -3.219 4.337 1.00 0.00 C ATOM 450 O GLY A 34144.841 -2.978 3.884 1.00 0.00 O **ATOM** 451 H GLY A 34145.029 -5.181 2.883 1.00 0.00 H ATOM 452 1HA GLY A 34147.273 -4.856 4.684 1.00 0.00 H ATOM 453 2HA GLY A 34147.476 -4.081 3.121 1.00 0.00 H ATOM ATOM 454 N VALA 35146.541 -2.468 5.266 1.00 0.00 N

455 CA VAL A 35145.884 -1.291 5.818 1.00 0.00 C ATOM 456 C VALA 35146.524 -0.008 5.294 1.00 0.00 C ATOM 457 O VALA 35147.743 0.072 5.144 1.00 0.00 O ATOM 458 CB VALA 35145.936 -1.289 7.360 1.00 0.00 C ATOM 459 CG1 VAL A 35147.377 -1.253 7.849 1.00 0.00 C ATOM 460 CG2 VAL A 35145.140 -0.120 7.925 1.00 0.00 C ATOM 461 H VALA 35147.434 -2.712 5.588 1.00 0.00 H **ATOM** 462 HA VALA 35144.848 -1.314 5.514 1.00 0.00 H ATOM 463 HB VALA 35145.486 -2.206 7.713 1.00 0.00 H **ATOM** 464 1HG1 VAL A 35147.393 -1.031 8.905 1.00 0.00 H ATOM 465 2HG1 VAL A 35147.920 -0.489 7.312 1.00 0.00 H **ATOM** 466 3HG1 VAL A 35147.841 -2.213 7.675 1.00 0.00 H ATOM 467 1HG2 VAL A 35144.771 0.491 7.115 1.00 0.00 H **ATOM** 468 2HG2 VAL A 35145.777 0.476 8.563 1.00 0.00 H ATOM 469 3HG2 VAL A 35144.307 -0.497 8.500 1.00 0.00 H ATOM 470 N ILE A 36145.694 0.991 5.016 1.00 0.00 N ATOM 471 CA ILE A 36146.181 2.269 4.508 1.00 0.00 C **ATOM** 472 C ILE A 36147.115 2.937 5.513 1.00 0.00 C **ATOM** 473 O ILE A 36146.824 2.986 6.708 1.00 0.00 O ATOM 474 CB ILE A 36145.017 3.229 4.186 1.00 0.00 C ATOM 475 CG1 ILE A 36143.994 2.541 3.278 1.00 0.00 C **ATOM** ATOM 476 CG2 ILE A 36145.541 4.501 3.533 1.00 0.00 C 477 CD1 ILE A 36142.827 3.428 2.903 1.00 0.00 C ATOM 478 H ILEA 36144.733 0.868 5.157 1.00 0.00 H **ATOM** 479 HA ILE A 36146.727 2.079 3.596 1.00 0.00 H ATOM 480 HB ILE A 36144.538 3.502 5.114 1.00 0.00 H **ATOM** 481 1HG1 ILE A 36144.482 2.233 2.367 1.00 0.00 H ATOM 482 2HG1 ILE A 36143.601 1.671 3.784 1.00 0.00 H ATOM 483 1HG2 ILE A 36145.386 4.447 2.465 1.00 0.00 H **ATOM** 484 2HG2 ILE A 36146.597 4.602 3.738 1.00 0.00 H ATOM ATOM 485 3HG2 ILE A 36145.013 5.354 3.931 1.00 0.00 H

486 1HD1 ILE A 36142.347 3.036 2.018 1.00 0.00 H **ATOM** 487 2HD1 ILE A 36143.183 4.428 2.706 1.00 0.00 H **ATOM** 488 3HD1 ILE A 36142.116 3.452 3.716 1.00 0.00 H **ATOM** 489 N ARG A 37148.237 3.449 5.019 1.00 0.00 N **ATOM** 490 CA ARG A 37149.215 4.113 5.872 1.00 0.00 C **ATOM** 491 C ARG A 37149.395 5.571 5.462 1.00 0.00 C **ATOM** 492 O ARG A 37149.097 6.483 6.232 1.00 0.00 O ATOM 493 CB ARG A 37150.558 3.383 5.807 1.00 0.00 C ATOM 494 CG ARG A 37150.462 1.902 6.127 1.00 0.00 C ATOM 495 CD ARG A 37149.957 1.669 7.543 1.00 0.00 C **ATOM** 496 NE ARG A 37150.921 2.111 8.547 1.00 0.00 N ATOM 497 CZ ARG A 37150.615 2.326 9.825 1.00 0.00 C ATOM 498 NH1 ARG A 37149.373 2.142 10.257 1.00 0.00 N ATOM 499 NH2 ARG A 37151.552 2.726 10.673 1.00 0.00 N ATOM 500 H ARG A 37148.412 3.377 4.057 1.00 0.00 H ATOM 501 HA ARG A 37148.847 4.080 6.887 1.00 0.00 H **ATOM** 502 1HB ARG A 37150.964 3.489 4.811 1.00 0.00 H ATOM 503 2HB ARG A 37151.237 3.839 6.513 1.00 0.00 H ATOM 504 1HG ARG A 37149.779 1.436 5.432 1.00 0.00 H **ATOM** 505 2HG ARGA 37151.441 1.457 6.027 1.00 0.00 H ATOM 506 1HD ARG A 37149.036 2.217 7.676 1.00 0.00 H **ATOM** 507 2HD ARG A 37149.770 0.614 7.675 1.00 0.00 H **ATOM** 508 HE ARG A 37151.845 2.255 8.255 1.00 0.00 H **ATOM** 509 1HH1 ARG A 37148.661 1.839 9.623 1.00 0.00 H **ATOM** 510 2HH1 ARG A 37149.150 2.304 11.218 1.00 0.00 H **ATOM** 511 1HH2 ARG A 37152.488 2.866 10.352 1.00 0.00 H **ATOM** 512 2HH2 ARG A 37151.322 2.887 11.632 1.00 0.00 H ATOM 513 N TRP A 38149.882 5.784 4.244 1.00 0.00 N ATOM 514 CA TRPA 38150.100 7.132 3.733 1.00 0.00 C ATOM 515 C TRPA 38149.375 7.336 2.406 1.00 0.00 C **ATOM** 516 O TRP A 38149.482 6.516 1.495 1.00 0.00 O

517 CB TRPA 38151.599 7.402 3.559 1.00 0.00 C 518 CG TRPA 38151.898 8.654 2.788 1.00 0.00 C ATOM 519 CD1 TRP A 38152.099 9.904 3.297 1.00 0.00 C **ATOM** 520 CD2 TRP A 38152.022 8.774 1.366 1.00 0.00 C **ATOM** 521 NE1 TRP A 38152.341 10.795 2.279 1.00 0.00 N ATOM **ATOM** 522 CE2 TRP A 38152.299 10.126 1.084 1.00 0.00 C 523 CE3 TRP A 38151.926 7.871 0.304 1.00 0.00 C **ATOM** 524 CZ2 TRP A 38152.481 10.593 -0.216 1.00 0.00 C ATOM 525 CZ3 TRP A 38152.107 8.335 -0.985 1.00 0.00 C ATOM 526 CH2 TRP A 38152.381 9.685 -1.236 1.00 0.00 C ATOM 527 H TRPA 38150.101 5.016 3.675 1.00 0.00 H ATOM 528 HA TRP A 38149.700 7.828 4.456 1.00 0.00 H **ATOM** 529 1HB TRP A 38152.056 7.494 4.533 1.00 0.00 H **ATOM** 530 2HB TRP A 38152.049 6.571 3.035 1.00 0.00 H **ATOM** 531 HD1 TRP A 38152.068 10.144 4.350 1.00 0.00 H ATOM 532 HE1 TRP A 38152.516 11.753 2.391 1.00 0.00 H **ATOM** 533 HE3 TRP A 38151.715 6.827 0.477 1.00 0.00 H **ATOM** 534 HZ2 TRP A 38152.690 11.631 -0.427 1.00 0.00 H **ATOM** 535 HZ3 TRP A 38152.037 7.652 -1.818 1.00 0.00 H **ATOM** ATOM 536 HH2 TRP A 38152.516 10.004 -2.259 1.00 0.00 H 537 N ILE A 39148.646 8.442 2.303 1.00 0.00 N **ATOM** 538 CA ILE A 39147.911 8.766 1.088 1.00 0.00 C **ATOM** 539 C ILE A 39148.340 10.125 0.546 1.00 0.00 C **ATOM** 540 O ILEA 39147.988 11.165 1.104 1.00 0.00 O **ATOM** 541 CB ILE A 39146.391 8.780 1.335 1.00 0.00 C ATOM 542 CG1 ILE A 39145.961 7.521 2.089 1.00 0.00 C **ATOM** 543 CG2 ILE A 39145.640 8.896 0.016 1.00 0.00 C ATOM 544 CD1 ILE A 39144.572 7.613 2.680 1.00 0.00 C ATOM 545 H ILE A 39148,608 9.060 3.063 1.00 0.00 H **ATOM** 546 HA ILE A 39148.130 8.008 0.350 1.00 0.00 H ATOM ATOM 547 HB ILE A 39146.153 9.647 1.932 1.00 0.00 H

548 1HG1 ILE A 39145.977 6.680 1.411 1.00 0.00 H ATOM 549 2HG1 ILE A 39146.656 7.338 2.897 1.00 0.00 H **ATOM** 550 1HG2 ILE A 39144.577 8.847 0.202 1.00 0.00 H **ATOM** 551 2HG2 ILE A 39145.930 8.085 -0.636 1.00 0.00 H **ATOM** 552 3HG2 ILE A 39145.880 9.839 -0.453 1.00 0.00 H ATOM 553 1HD1 ILE A 39143.973 8.287 2.086 1.00 0.00 H ATOM ATOM 554 2HD1 ILE A 39144.635 7.984 3.692 1.00 0.00 H 555 3HD1 ILE A 39144.116 6.634 2.682 1.00 0.00 H **ATOM** 556 N GLY A 40149.108 10.112 -0.539 1.00 0.00 N **ATOM** 557 CA GLY A 40149.576 11.353 -1.126 1.00 0.00 C ATOM 558 C GLY A 40150.128 11.169 -2.526 1.00 0.00 C **ATOM ATOM** 559 O GLY A 40149.973 10.107 -3.129 1.00 0.00 O 560 H GLY A 40149.362 9.254 -0.940 1.00 0.00 H **ATOM** 561 1HA GLY A 40148.755 12.052 -1.165 1.00 0.00 H **ATOM** 562 2HA GLY A 40150.351 11.763 -0.498 1.00 0.00 H **ATOM** 563 N GLN A 41150.772 12.210 -3.042 1.00 0.00 N **ATOM** 564 CA GLN A 41151.352 12.170 -4.378 1.00 0.00 C **ATOM** 565 C GLN A 41152.824 12.581 -4.341 1.00 0.00 C **ATOM** 566 O GLN A 41153.146 13.724 -4.012 1.00 0.00 O ATOM 567 CB GLN A 41150.574 13.098 -5.310 1.00 0.00 C ATOM 568 CG GLN A 41149.068 12.908 -5.240 1.00 0.00 C ATOM 569 CD GLN A 41148.312 14.221 -5.293 1.00 0.00 C **ATOM** 570 OE1 GLN A 41148.274 14.968 -4.315 1.00 0.00 O **ATOM** 571 NE2 GLN A 41147.705 14.509 -6.437 1.00 0.00 N ATOM 572 H GLN A 41150.861 13.027 -2.510 1.00 0.00 H **ATOM** 573 HA GLN A 41151.277 11.159 -4.745 1.00 0.00 H **ATOM** 574 1HB GLN A 41150.798 14.121 -5.048 1.00 0.00 H **ATOM** 575 2HB GLN A 41150.892 12.919 -6.325 1.00 0.00 H **ATOM** 576 1HG GLN A 41148.754 12.298 -6.074 1.00 0.00 H **ATOM** 577 2HG GLN A 41148.824 12.406 -4.316 1.00 0.00 H **ATOM** 578 1HE2 GLN A 41147.778 13.866 -7.174 1.00 0.00 H ATOM

ATOM 579 2HE2 GLN A 41147.211 15.351 -6.500 1.00 0.00 H 580 N PRO A 42153.742 11.656 -4.675 1.00 0.00 N 581 CA PRO A 42155.181 11.939 -4.673 1.00 0.00 C ATOM 582 C PRO A 42155.542 13.108 -5.584 1.00 0.00 C ATOM 583 O PRO A 42154.782 13.461 -6.486 1.00 0.00 O ATOM 584 CB PRO A 42155.808 10.641 -5.194 1.00 0.00 C ATOM 585 CG PRO A 42154.786 9.590 -4.928 1.00 0.00 C ATOM 586 CD PRO A 42153.455 10.268 -5.079 1.00 0.00 C ATOM 587 HA PRO A 42155.542 12.139 -3.674 1.00 0.00 H ATOM **ATOM** 588 1HB PRO A 42156.012 10.737 -6.250 1.00 0.00 H ATOM 589 2HB PRO A 42156.725 10.442 -4.661 1.00 0.00 H **ATOM** 590 1HG PRO A 42154.883 8.791 -5.647 1.00 0.00 H 591 2HG PRO A 42154.901 9.210 -3.923 1.00 0.00 H ATOM 592 1HD PRO A 42153.124 10.226 -6.107 1.00 0.00 H ATOM 593 2HD PRO A 42152.724 9.819 -4.424 1.00 0.00 H ATOM 594 N PRO A 43156.714 13.726 -5.360 1.00 0.00 N ATOM ATOM 595 CA PRO A 43157.174 14.860 -6.166 1.00 0.00 C ATOM 596 C PRO A 43157.596 14.441 -7.569 1.00 0.00 C 597 O PROA 43158.768 14.155 -7.816 1.00 0.00 O ATOM 598 CB PRO A 43158.377 15.386 -5.384 1.00 0.00 C ATOM 599 CG PRO A 43158.887 14.204 -4.634 1.00 0.00 C **ATOM** 600 CD PRO A 43157.681 13.366 -4.305 1.00 0.00 C ATOM 601 HA PRO A 43156.419 15.630 -6.233 1.00 0.00 H **ATOM** 602 1HB PRO A 43159.117 15.767 -6.073 1.00 0.00 H ATOM 603 2HB PRO A 43158.061 16.171 -4.714 1.00 0.00 H **ATOM** 604 1HG PRO A 43159.573 13.646 -5.253 1.00 0.00 H ATOM 605 2HG PRO A 43159.376 14.528 -3.728 1.00 0.00 H **ATOM** 606 1HD PRO A 43157.928 12.316 -4.350 1.00 0.00 H ATOM 607 2HD PRO A 43157.298 13.624 -3.329 1.00 0.00 H ATOM 608 N GLY A 44156.635 14.406 -8.486 1.00 0.00 N ATOM ATOM 609 CA GLY A 44156.931 14.021 -9.852 1.00 0.00 C

- ATOM 610 C GLY A 44155.710 13.511 -10.590 1.00 0.00 C
- ATOM 611 O GLY A 44155.412 13.962 -11.696 1.00 0.00 O
- ATOM 612 H GLY A 44155.719 14.645 -8.232 1.00 0.00 H
- ATOM 613 1HA GLY A 44157.323 14.877 -10.378 1.00 0.00 H
- ATOM 614 2HA GLY A 44157.681 13.245 -9.840 1.00 0.00 H
- ATOM 615 N LEU A 45155.002 12.568 -9.979 1.00 0.00 N
- ATOM 616 CA LEU A 45153.807 11.996 -10.589 1.00 0.00 C
- ATOM 617 C LEUA 45152.592 12.203 -9.694 1.00 0.00 C
- ATOM 618 O LEU A 45152.501 11.623 -8.612 1.00 0.00 O
- ATOM 619 CB LEU A 45154.011 10.504 -10.858 1.00 0.00 C
- ATOM 620 CG LEU A 45154.560 9.704 -9.674 1.00 0.00 C
- ATOM 621 CD1 LEU A 45154.219 8.227 -9.821 1.00 0.00 C
- ATOM 622 CD2 LEU A 45156.066 9.899 -9.551 1.00 0.00 C
- ATOM 623 H LEU A 45155.289 12.247 -9.096 1.00 0.00 H
- ATOM 624 HA LEU A 45153.640 12.503 -11.528 1.00 0.00 H
- ATOM 625 1HB LEU A 45153.060 10.079 -11.144 1.00 0.00 H
- ATOM 626 2HB LEU A 45154.698 10.399 -11.684 1.00 0.00 H
- ATOM 627 HG LEU A 45154.101 10.062 -8.764 1.00 0.00 H
- ATOM 628 1HD1 LEU A 45153.622 8.081 -10.710 1.00 0.00 H
- ATOM 629 2HD1 LEU A 45153.661 7.900 -8.956 1.00 0.00 H
- ATOM 630 3HD1 LEU A 45155.130 7.652 -9.900 1.00 0.00 H
- ATOM 631 1HD2 LEU A 45156.572 8.983 -9.824 1.00 0.00 H
- ATOM 632 2HD2 LEU A 45156.312 10.155 -8.530 1.00 0.00 H
- ATOM 633 3HD2 LEU A 45156.383 10.694 -10.208 1.00 0.00 H
- ATOM 634 N ASN A 46151.656 13.030 -10.149 1.00 0.00 N
- ATOM 635 CA ASN A 46150.449 13.299 -9.377 1.00 0.00 C
- ATOM 636 C ASN A 46149.512 12.098 -9.414 1.00 0.00 C
- ATOM 637 O ASN A 46148.893 11.810 -10.438 1.00 0.00 O
- ATOM 638 CB ASN A 46149.736 14.537 -9.925 1.00 0.00 C
- ATOM 639 CG ASN A 46148.974 15.289 -8.852 1.00 0.00 C
- ATOM 640 OD1 ASN A 46147.746 15.375 -8.891 1.00 0.00 O

641 ND2 ASN A 46149.700 15.838 -7.884 1.00 0.00 N 642 H ASN A 46151.778 13.465 -11.018 1.00 0.00 H **ATOM** · ATOM 643 HA ASN A 46150.742 13.484 -8.355 1.00 0.00 H 644 1HB ASN A 46150.466 15.205 -10.356 1.00 0.00 H ATOM **ATOM** 645 2HB ASN A 46149.038 14.232 -10.691 1.00 0.00 H 646 1HD2 ASN A 46150.673 15.727 -7.917 1.00 0.00 H ATOM **ATOM** 647 2HD2 ASN A 46149.233 16.329 -7.178 1.00 0.00 H 648 N GLUA 47149.415 11.401 -8.288 1.00 0.00 N **ATOM** 649 CA GLUA 47148.555 10.230 -8.183 1.00 0.00 C **ATOM ATOM** 650 C GLUA 47148.375 9.820 -6.726 1.00 0.00 C 651 O GLUA 47149.348 9.519 -6.034 1.00 0.00 O ATOM ATOM 652 CB GLU A 47149.138 9.063 -8.985 1.00 0.00 C 653 CG GLUA 47150.653 8.959 -8.902 1.00 0.00 C ATOM 654 CD GLU A 47151.235 8.068 -9.981 1.00 0.00 C **ATOM** 655 OE1 GLU A 47151.350 8.531 -11.134 1.00 0.00 O **ATOM** 656 OE2 GLU A 47151.575 6.905 -9.672 1.00 0.00 O **ATOM** ATOM 657 H GLUA 47149.935 11.682 -7.507 1.00 0.00 H **ATOM** 658 HA GLUA 47147.590 10.490 -8.592 1.00 0.00 H 659 1HB GLU A 47148.715 8.141 -8.616 1.00 0.00 H ATOM 660 2HB GLU A 47148.864 9.183 -10.022 1.00 0.00 H **ATOM** 661 1HG GLU A 47151.075 9.946 -9.006 1.00 0.00 H **ATOM** 662 2HG GLUA 47150.922 8.554 -7.937 1.00 0.00 H **ATOM** 663 N VALA 48147.130 9.802 -6.264 1.00 0.00 N ATOM 664 CA VALA 48146.839 9.420 -4.889 1.00 0.00 C ATOM 665 C VALA 48147.232 7.969 -4.639 1.00 0.00 C ATOM 666 O VALA 48146.502 7.047 -5.001 1.00 0.00 O ATOM 667 CB VAL A 48145.346 9.605 -4.557 1.00 0.00 C **ATOM** 668 CG1 VAL A 48145.100 9.395 -3.071 1.00 0.00 C **ATOM** 669 CG2 VAL A 48144.867 10.980 -4.996 1.00 0.00 C ATOM 670 H VALA 48146.393 10.047 -6.862 1.00 0.00 H ATOM

671 HA VALA 48147.417 10.058 -4.236 1.00 0.00 H

672 HB VALA 48144.783 8.860 -5.100 1.00 0.00 H ATOM 673 1HG1 VAL A 48144.082 9.666 -2.834 1.00 0.00 H **ATOM** 674 2HG1 VAL A 48145.780 10.014 -2.503 1.00 0.00 H ATOM 675 3HG1 VAL A 48145.265 8.358 -2.821 1.00 0.00 H ATOM 676 1HG2 VAL A 48145.704 11.662 -5.017 1.00 0.00 H **ATOM** 677 2HG2 VAL A 48144.125 11.342 -4.301 1.00 0.00 H ATOM 678 3HG2 VAL A 48144.433 10.912 -5.983 1.00 0.00 H ATOM 679 N LEUA 49148.392 7.774 -4.021 1.00 0.00 N ATOM 680 CA LEU A 49148.884 6.434 -3.727 1.00 0.00 C ATOM 681 C LEUA 49148.782 6.135 -2.237 1.00 0.00 C ATOM 682 O LEUA 49149.437 6.780 -1.418 1.00 0.00 O **ATOM** 683 CB LEUA 49150.333 6.286 -4.190 1.00 0.00 C **ATOM** 684 CG LEUA 49150.544 6.396 -5.702 1.00 0.00 C **ATOM** 685 CD1 LEU A 49151.921 6.965 -6.009 1.00 0.00 C **ATOM** 686 CD2 LEU A 49150.367 5.038 -6.363 1.00 0.00 C ATOM **ATOM** 687 H LEUA 49148.932 8.549 -3.758 1.00 0.00 H 688 HA LEUA 49148.269 5.729 -4.266 1.00 0.00 H ATOM 689 1HB LEU A 49150.924 7.053 -3.709 1.00 0.00 H **ATOM** 690 2HB LEU A 49150.696 5.322 -3.869 1.00 0.00 H ATOM 691 HG LEUA 49149.806 7.068 -6.114 1.00 0.00 H **ATOM** 692 1HD1 LEU A 49151.845 8.033 -6.150 1.00 0.00 H **ATOM** 693 2HD1 LEU A 49152.306 6.509 -6.908 1.00 0.00 H **ATOM** 694 3HD1 LEU A 49152.588 6.757 -5.186 1.00 0.00 H ATOM 695 1HD2 LEU A 49151.056 4.331 -5.924 1.00 0.00 H ATOM 696 2HD2 LEU A 49150.566 5.123 -7.421 1.00 0.00 H ATOM 697 3HD2 LEU A 49149.354 4.694 -6.214 1.00 0.00 H **ATOM** 698 N ALAA 50147.954 5.157 -1.890 1.00 0.00 N **ATOM** 699 CA ALAA 50147.767 4.778 -0.498 1.00 0.00 C **ATOM** 700 C ALAA 50148.728 3.663 -0.099 1.00 0.00 C **ATOM** 701 O ALAA 50148.645 2.546 -0.611 1.00 0.00 O **ATOM** 702 CB ALAA 50146.329 4.352 -0.254 1.00 0.00 C ATOM

ATOM 703 H ALAA 50147.457 4.680 -2.588 1.00 0.00 H 704 HA ALAA 50147.968 5.649 0.110 1.00 0.00 H **ATOM** 705 1HB ALA A 50146.304 3.578 0.500 1.00 0.00 H **ATOM** 706 2HB ALA A 50145.905 3.973 -1.172 1.00 0.00 H **ATOM** 707 3HB ALA A 50145.753 5.201 0.084 1.00 0.00 H ATOM 708 N GLY A 51149.639 3.971 0.818 1.00 0.00 N **ATOM** 709 CA GLY A 51150.601 2.984 1.269 1.00 0.00 C **ATOM** 710 C GLYA 51149.968 1.910 2.133 1.00 0.00 C **ATOM** 711 O GLY A 51149.673 2.142 3.305 1.00 0.00 O **ATOM** 712 H GLYA 51149.657 4.877 1.191 1.00 0.00 H **ATOM** 713 1HA GLY A 51151.053 2.516 0.406 1.00 0.00 H **ATOM** 714 2HA GLY A 51151.371 3.482 1.839 1.00 0.00 H ATOM 715 N LEUA 52149.760 0.733 1.554 1.00 0.00 N ATOM 716 CA LEU A 52149.158 -0.379 2.279 1.00 0.00 C **ATOM** 717 C LEU A 52150.226 -1.227 2.962 1.00 0.00 C ATOM 718 O LEUA 52151.311 -1.435 2.418 1.00 0.00 O **ATOM ATOM** 719 CB LEU A 52148.331 -1.247 1.329 1.00 0.00 C 720 CG LEU A 52147.092 -0.567 0.742 1.00 0.00 C ATOM 721 CD1 LEU A 52146.492 -1.417 -0.367 1.00 0.00 C **ATOM** 722 CD2 LEU A 52146.064 -0.305 1.832 1.00 0.00 C **ATOM** 723 H LEU A 52150.018 0.609 0.617 1.00 0.00 H **ATOM** 724 HA LEU A 52148.505 0.033 3.035 1.00 0.00 H **ATOM** 725 1HB LEU A 52148.968 -1.558 0.513 1.00 0.00 H **ATOM** 726 2HB LEU A 52148.010 -2.127 1.866 1.00 0.00 H **ATOM** 727 HG LEU A 52147.380 0.383 0.317 1.00 0.00 H **ATOM** 728 1HD1 LEU A 52146.896 -1.104 -1.319 1.00 0.00 H ATOM 729 2HD1 LEU A 52145.420 -1.294 -0.374 1.00 0.00 H **ATOM** 730 3HD1 LEU A 52146.736 -2.456 -0.197 1.00 0.00 H ATOM 731 1HD2 LEU A 52146.171 -1.044 2.613 1.00 0.00 H **ATOM** 732 2HD2 LEU A 52145.071 -0.367 1.412 1.00 0.00 H **ATOM** 733 3HD2 LEU A 52146.220 0.680 2.245 1.00 0.00 H ATOM

734 N GLUA 53149.911 -1.716 4.157 1.00 0.00 N **ATOM** 735 CA GLU A 53150.842 -2.542 4.916 1.00 0.00 C **ATOM** 736 C GLUA 53150.337 -3.977 5.018 1.00 0.00 C **ATOM** 737 O GLUA 53149.366 -4.256 5.720 1.00 0.00 O **ATOM** 738 CB GLU A 53151.049 -1.961 6.316 1.00 0.00 C **ATOM ATOM** 739 CG GLU A 53152.034 -2.750 7.163 1.00 0.00 C 740 CD GLUA 53151.587 -2.881 8.606 1.00 0.00 C ATOM 741 OE1 GLU A 53152.298 -2.368 9.497 1.00 0.00 O **ATOM** 742 OE2 GLU A 53150.528 -3.497 8.845 1.00 0.00 O **ATOM** 743 H GLUA 53149.031 -1.515 4.539 1.00 0.00 H **ATOM** 744 HA GLU A 53151.787 -2.541 4.393 1.00 0.00 H ATOM 745 1HB GLU A 53151.416 -0.950 6.224 1.00 0.00 H **ATOM** 746 2HB GLU A 53150.099 -1.944 6.830 1.00 0.00 H ATOM 747 1HG GLU A 53152.138 -3.739 6.743 1.00 0.00 H **ATOM ATOM** 748 2HG GLUA 53152.990 -2.248 7.141 1.00 0.00 H 749 N LEUA 54151.003 -4.885 4.310 1.00 0.00 N **ATOM** 750 CA LEUA 54150.620 -6.292 4.319 1.00 0.00 C **ATOM** 751 C LEUA 54150.836 -6.904 5.700 1.00 0.00 C **ATOM** 752 O LEUA 54151.871 -6.692 6.329 1.00 0.00 O **ATOM** 753 CB LEU A 54151.423 -7.067 3.273 1.00 0.00 C **ATOM** 754 CG LEUA 54151.413 -6.460 1.869 1.00 0.00 C **ATOM** 755 CD1 LEU A 54152.554 -7.023 1.036 1.00 0.00 C **ATOM** 756 CD2 LEU A 54150.076 -6.717 1.189 1.00 0.00 C **ATOM** 757 H LEUA 54151.769 -4.601 3.768 1.00 0.00 H **ATOM** 758 HA LEU A 54149.571 -6.352 4.072 1.00 0.00 H **ATOM** 759 1HB LEU A 54152.448 -7.128 3.610 1.00 0.00 H **ATOM** 760 2HB LEU A 54151.022 -8.068 3.211 1.00 0.00 H **ATOM** 761 HG LEU A 54151.551 -5.392 1.944 1.00 0.00 H **ATOM** 762 1HD1 LEU A 54152.684 -8.071 1.266 1.00 0.00 H **ATOM** 763 2HD1 LEU A 54153.463 -6.489 1.263 1.00 0.00 H **ATOM** 764 3HD1 LEU A 54152.323 -6.911 -0.013 1.00 0.00 H ATOM

765 1HD2 LEU A 54149.629 -7.612 1.599 1.00 0.00 H **ATOM ATOM** 766 2HD2 LEU A 54150.230 -6.846 0.128 1.00 0.00 H 767 3HD2 LEU A 54149.419 -5.877 1.357 1.00 0.00 H ATOM **ATOM** 768 N GLUA 55149.850 -7.665 6.164 1.00 0.00 N **ATOM** 769 CA GLU A 55149.930 -8.310 7.469 1.00 0.00 C 770 C GLUA 55151.044 -9.351 7.494 1.00 0.00 C **ATOM** 771 O GLUA 55151.685 -9.565 8.524 1.00 0.00 O ATOM 772 CB GLU A 55148.594 -8.967 7.822 1.00 0.00 C **ATOM** 773 CG GLU A 55147.552 -7.987 8.337 1.00 0.00 C **ATOM** 774 CD GLUA 55146.137 -8.398 7.975 1.00 0.00 C ATOM 775 OE1 GLU A 55145.968 -9.127 6.975 1.00 0.00 O **ATOM** 776 OE2 GLU A 55145.200 -7.990 8.692 1.00 0.00 O ATOM ATOM 777 H GLUA 55149.048 -7.797 5.615 1.00 0.00 H 778 HA GLU A 55150.150 -7.547 8.202 1.00 0.00 H ATOM **ATOM** 779 1HB GLU A 55148.199 -9.448 6.939 1.00 0.00 H 780 2HB GLU A 55148.763 -9.712 8.584 1.00 0.00 H ATOM 781 1HG GLUA 55147.630 -7.930 9.412 1.00 0.00 H **ATOM** ATOM 782 2HG GLU A 55147.749 -7.015 7.910 1.00 0.00 H 783 N ASPA 56151.269 -9.997 6.356 1.00 0.00 N ATOM 784 CA ASPA 56152.306 -11.017 6.248 1.00 0.00 C ATOM 785 C ASP A 56153.580 -10.435 5.642 1.00 0.00 C **ATOM** 786 O ASPA 56153.529 -9.483 4.864 1.00 0.00 O ATOM 787 CB ASP A 56151.812 -12.189 5.397 1.00 0.00 C **ATOM ATOM** 788 CG ASP A 56150.930 -13.140 6.180 1.00 0.00 C 789 OD1 ASP A 56149.691 -13.034 6.064 1.00 0.00 O ATOM 790 OD2 ASP A 56151.478 -13.993 6.910 1.00 0.00 O **ATOM** 791 H ASPA 56150.725 -9.784 5.569 1.00 0.00 H ATOM 792 HA ASP A 56152.526 -11.374 7.243 1.00 0.00 H ATOM 793 1HB ASP A 56151.244 -11.805 4.563 1.00 0.00 H **ATOM** 794 2HB ASP A 56152.664 -12.739 5.024 1.00 0.00 H **ATOM** 795 N GLUA 57154.719 -11.014 6.006 1.00 0.00 N ATOM

796 CA GLUA 57156.006 -10.552 5.498 1.00 0.00 C 797 C GLUA 57156.353 -11.245 4.184 1.00 0.00 C **ATOM** 798 O GLUA 57156.738 -12.414 4.170 1.00 0.00 O ATOM 799 CB GLUA 57157.107 -10.810 6.529 1.00 0.00 C **ATOM** 800 CG GLU A 57157.130 -9.795 7.660 1.00 0.00 C ATOM 801 CD GLUA 57158.393 -9.882 8.496 1.00 0.00 C ATOM **ATOM** 802 OE1 GLU A 57158.992 -10.976 8.553 1.00 0.00 O 803 OE2 GLU A 57158.782 -8.856 9.092 1.00 0.00 O ATOM 804 H GLUA 57154.694 -11.769 6.630 1.00 0.00 H **ATOM** 805 HA GLUA 57155.932 -9.490 5.323 1.00 0.00 H ATOM 806 1HB GLU A 57156.960 -11.791 6.958 1.00 0.00 H **ATOM** 807 2HB GLUA 57158.064 -10.784 6.031 1.00 0.00 H **ATOM** 808 1HG GLU A 57157.065 -8.803 7.238 1.00 0.00 H **ATOM** 809 2HG GLUA 57156.278 -9.969 8.301 1.00 0.00 H ATOM 810 N CYS A 58156.214 -10.515 3.082 1.00 0.00 N ATOM 811 CA CYS A 58156.513 -11.058 1.762 1.00 0.00 C ATOM **ATOM** 812 C CYS A 58157.824 -10.492 1.225 1.00 0.00 C 813 O CYS A 58157.973 -9.279 1.077 1.00 0.00 O **ATOM** 814 CB CYS A 58155.374 -10.750 0.790 1.00 0.00 C **ATOM** 815 SG CYS A 58155.604 -11.445 -0.862 1.00 0.00 S ATOM 816 H CYS A 58155.904 -9.589 3.158 1.00 0.00 H **ATOM** 817 HA CYS A 58156.612 -12.129 1.860 1.00 0.00 H **ATOM** 818 1HB CYS A 58154.453 -11.150 1.188 1.00 0.00 H **ATOM** 819 2HB CYS A 58155.279 -9.678 0.687 1.00 0.00 H **ATOM** 820 HG CYS A 58156.540 -11.627 -0.979 1.00 0.00 H **ATOM** 821 N ALAA 59158.770 -11.378 0.933 1.00 0.00 N **ATOM** 822 CA ALA A 59160.067 -10.966 0.411 1.00 0.00 C **ATOM** 823 C ALAA 59159.915 -10.208 -0.903 1.00 0.00 C ATOM 824 O ALAA 59159.155 -10.615 -1.782 1.00 0.00 O **ATOM** 825 CB ALA A 59160.968 -12.177 0.223 1.00 0.00 C **ATOM** ATOM 826 H ALAA 59158.592 -12.331 1.071 1.00 0.00 H

- ATOM 827 HA ALA A 59160.528 -10.315 1.140 1.00 0.00 H ATOM 828 1HB ALA A 59160.734 -12.921 0.969 1.00 0.00 H
- ATOM 829 2HB ALA A 59162.001 -11.877 0.326 1.00 0.00 H
- ATOM 830 3HB ALA A 59160.811 -12.593 -0.762 1.00 0.00 H
- ATOM 831 N GLY A 60160.643 -9.103 -1.031 1.00 0.00 N
- ATOM 832 CA GLY A 60160.574 -8.305 -2.241 1.00 0.00 C
- ATOM 833 C GLY A 60160.044 -6.908 -1.985 1.00 0.00 C
- ATOM 834 O GLY A 60160.381 -5.967 -2.703 1.00 0.00 O
- ATOM 835 H GLY A 60161.231 -8.827 -0.298 1.00 0.00 H
- ATOM 836 1HA GLY A 60161.564 -8.229 -2.666 1.00 0.00 H
- ATOM 837 2HA GLY A 60159.927 -8.799 -2.951 1.00 0.00 H
- ATOM 838 N CYS A 61159.210 -6.773 -0.959 1.00 0.00 N
- ATOM 839 CA CYS A 61158.631 -5.480 -0.610 1.00 0.00 C
- ATOM 840 C CYS A 61159.598 -4.662 0.240 1.00 0.00 C
- ATOM 841 O CYS A 61160.705 -5.109 0.542 1.00 0.00 O
- ATOM 842 CB CYS A 61157.314 -5.675 0.143 1.00 0.00 C
- ATOM 843 SG CYS A 61156.183 -6.848 -0.641 1.00 0.00 S
- ATOM 844 H CYS A 61158.978 -7.560 -0.424 1.00 0.00 H
- ATOM 845 HA CYS A 61158.435 -4.946 -1.527 1.00 0.00 H
- ATOM 846 1HB CYS A 61157.525 -6.040 1.137 1.00 0.00 H
- ATOM 847 2HB CYS A 61156.804 -4.725 0.215 1.00 0.00 H
- ATOM 848 HG CYS A 61156.528 -7.057 -1.512 1.00 0.00 H
- ATOM 849 N THR A 62159.174 -3.462 0.620 1.00 0.00 N
- ATOM 850 CA THR A 62160.003 -2.581 1.435 1.00 0.00 C
- ATOM 851 C THR A 62159.434 -2.448 2.844 1.00 0.00 C
- ATOM 852 O THR A 62158.454 -3.106 3.192 1.00 0.00 O
- ATOM 853 CB THR A 62160.110 -1.201 0.784 1.00 0.00 C
- ATOM 854 OG1 THR A 62158.839 -0.580 0.714 1.00 0.00 O
- ATOM 855 CG2 THR A 62160.677 -1.243 -0.618 1.00 0.00 C
- ATOM 856 H THR A 62158.283 -3.161 0.347 1.00 0.00 H
- ATOM 857 HA THR A 62160.989 -3.017 1.497 1.00 0.00 H

858 HB THR A 62160.758 -0.580 1.385 1.00 0.00 H **ATOM** 859 HG1 THR A 62158.243 -1.125 0.195 1.00 0.00 H **ATOM** 860 1HG2 THR A 62160.591 -2.245 -1.011 1.00 0.00 H **ATOM** 861 2HG2 THR A 62161.718 -0.954 -0.595 1.00 0.00 H **ATOM** 862 3HG2 THR A 62160.128 -0.561 -1.250 1.00 0.00 H **ATOM ATOM** 863 N ASPA 63160.056 -1.594 3.649 1.00 0.00 N 864 CA ASP A 63159.612 -1.375 5.021 1.00 0.00 C **ATOM** 865 C ASPA 63158.866 -0.050 5.147 1.00 0.00 C **ATOM ATOM** 866 O ASPA 63158.935 0.616 6.180 1.00 0.00 O 867 CB ASP A 63160.806 -1.393 5.976 1.00 0.00 C **ATOM** 868 CG ASP A 63161.904 -0.439 5.547 1.00 0.00 C **ATOM** 869 OD1 ASP A 63162.936 -0.917 5.028 1.00 0.00 O ATOM 870 OD2 ASP A 63161.732 0.784 5.729 1.00 0.00 O ATOM 871 H ASPA 63160.832 -1.098 3.314 1.00 0.00 H ATOM 872 HA ASP A 63158.940 -2.178 5.284 1.00 0.00 H **ATOM** 873 1HB ASP A 63160.475 -1.110 6.963 1.00 0.00 H **ATOM** 874 2HB ASP A 63161.216 -2.393 6.011 1.00 0.00 H ATOM 875 N GLY A 64158.156 0.325 4.089 1.00 0.00 N ATOM 876 CA GLY A 64157.408 1.569 4.101 1.00 0.00 C ATOM 877 C GLY A 64158.144 2.695 3.402 1.00 0.00 C ATOM 878 O GLYA 64158.130 3.836 3.864 1.00 0.00 O **ATOM** 879 H GLY A 64158.138 -0.246 3.293 1.00 0.00 H ATOM 880 1HA GLYA 64156.460 1.412 3.608 1.00 0.00 H **ATOM** 881 2HA GLY A 64157.225 1.856 5.126 1.00 0.00 H **ATOM** 882 N THR A 65158.787 2.375 2.284 1.00 0.00 N **ATOM** 883 CA THR A 65159.532 3.367 1.519 1.00 0.00 C ATOM 884 C THR A 65159.121 3.343 0.051 1.00 0.00 C **ATOM** 885 O THR A 65159.276 2.330 -0.631 1.00 0.00 O ATOM 886 CB THR A 65161.036 3.116 1.644 1.00 0.00 C **ATOM** 887 OG1 THR A 65161.300 1.733 1.811 1.00 0.00 O **ATOM**

ATOM 888 CG2 THR A 65161.670 3.849 2.806 1.00 0.00 C

889 H THR A 65158.760 1.448 1.967 1.00 0.00 H ATOM 890 HA THR A 65159.304 4.341 1.929 1.00 0.00 H ATOM **ATOM** 891 HB THR A 65161.522 3.447 0.738 1.00 0.00 H 892 HG1 THR A 65161.736 1.394 1.027 1.00 0.00 H **ATOM** 893 1HG2 THR A 65161.388 3.369 3.731 1.00 0.00 H **ATOM** 894 2HG2 THR A 65161.331 4.874 2.813 1.00 0.00 H **ATOM** 895 3HG2 THR A 65162.745 3.826 2.702 1.00 0.00 H **ATOM** 896 N PHE A 66158.597 4.466 -0.431 1.00 0.00 N **ATOM** 897 CA PHE A 66158.164 4.572 -1.819 1.00 0.00 C **ATOM** 898 C PHE A 66159.235 5.243 -2.672 1.00 0.00 C **ATOM** 899 O PHE A 66159.380 6.465 -2.657 1.00 0.00 O **ATOM** 900 CB PHE A 66156.857 5.362 -1.909 1.00 0.00 C ATOM **ATOM** 901 CG PHE A 66156.098 5.124 -3.184 1.00 0.00 C 902 CD1 PHE A 66155.827 3.835 -3.613 1.00 0.00 C **ATOM** 903 CD2 PHE A 66155.657 6.190 -3.951 1.00 0.00 C ATOM 904 CE1 PHE A 66155.130 3.613 -4.786 1.00 0.00 C ATOM 905 CE2 PHE A 66154.959 5.974 -5.125 1.00 0.00 C ATOM 906 CZ PHE A 66154.695 4.684 -5.542 1.00 0.00 C ATOM 907 H PHE A 66158.499 5.240 0.162 1.00 0.00 H ATOM 908 HA PHE A 66157.997 3.574 -2.192 1.00 0.00 H **ATOM** 909 1HB PHE A 66156.218 5.082 -1.085 1.00 0.00 H **ATOM** 910 2HB PHE A 66157.078 6.417 -1.844 1.00 0.00 H **ATOM** 911 HD1 PHE A 66156.166 2.997 -3.022 1.00 0.00 H ATOM 912 HD2 PHE A 66155.863 7.198 -3.626 1.00 0.00 H **ATOM** 913 HE1 PHE A 66154.926 2.603 -5.111 1.00 0.00 H ATOM 914 HE2 PHE A 66154.621 6.812 -5.715 1.00 0.00 H **ATOM** 915 HZ PHE A 66154.150 4.514 -6.459 1.00 0.00 H **ATOM** 916 N ARG A 67159.983 4.435 -3.417 1.00 0.00 N **ATOM** 917 CA ARG A 67161.042 4.949 -4.278 1.00 0.00 C ATOM 918 C ARGA 67162.083 5.713 -3.465 1.00 0.00 C ATOM ATOM 919 O ARG A 67162.723 6.636 -3.969 1.00 0.00 O

920 CB ARG A 67160.453 5.860 -5.357 1.00 0.00 C 921 CG ARG A 67159.223 5.281 -6.038 1.00 0.00 C **ATOM** 922 CD ARG A 67158.382 6.368 -6.687 1.00 0.00 C **ATOM** 923 NE ARG A 67157.338 5.813 -7.546 1.00 0.00 N ATOM 924 CZ ARG A 67157.567 5.297 -8.752 1.00 0.00 C **ATOM** 925 NH1 ARG A 67158.799 5.263 -9.244 1.00 0.00 N ATOM 926 NH2 ARG A 67156.561 4.814 -9.466 1.00 0.00 N **ATOM** 927 H ARG A 67159.819 3.469 -3.387 1.00 0.00 H **ATOM** 928 HA ARG A 67161.521 4.107 -4.753 1.00 0.00 H ATOM 929 1HB ARG A 67160.177 6.802 -4.906 1.00 0.00 H ATOM 930 2HB ARG A 67161.205 6.037 -6.112 1.00 0.00 H **ATOM** 931 1HG ARG A 67159.539 4.582 -6.797 1.00 0.00 H **ATOM** 932 2HG ARG A 67158.623 4.768 -5.300 1.00 0.00 H ATOM 933 1HD ARG A 67157.919 6.959 -5.910 1.00 0.00 H **ATOM** 934 2HD ARG A 67159.027 6.998 -7.281 1.00 0.00 H ATOM 935 HE ARG A 67156.419 5.826 -7.206 1.00 0.00 H **ATOM** 936 1HH1 ARG A 67159.562 5.625 -8.709 1.00 0.00 H ATOM 937 2HH1 ARG A 67158.964 4.873 -10.149 1.00 0.00 H ATOM 938 1HH2 ARG A 67155.630 4.837 -9.101 1.00 0.00 H **ATOM** 939 2HH2 ARG A 67156.731 4.426 -10.372 1.00 0.00 H **ATOM ATOM** 940 N GLY A 68162.246 5.323 -2.205 1.00 0.00 N 941 CA GLY A 68163.211 5.983 -1.344 1.00 0.00 C **ATOM** 942 C GLY A 68162.572 7.006 -0.425 1.00 0.00 C **ATOM** 943 O GLY A 68163.149 7.375 0.598 1.00 0.00 O ATOM 944 H GLY A 68161.708 4.581 -1.856 1.00 0.00 H **ATOM** 945 1HA GLY A 68163.709 5.237 -0.743 1.00 0.00 H ATOM 946 2HA GLY A 68163.946 6.480 -1.961 1.00 0.00 H **ATOM** 947 N THR A 69161.378 7.467 -0.787 1.00 0.00 N **ATOM** 948 CA THR A 69160.666 8.455 0.015 1.00 0.00 C **ATOM** 949 C THR A 69159.834 7.778 1.100 1.00 0.00 C ATOM 950 O THR A 69158.714 7.331 0.851 1.00 0.00 O

ATOM

951 CB THR A 69159.763 9.310 -0.875 1.00 0.00 C **ATOM** 952 OG1 THR A 69160.491 9.830 -1.974 1.00 0.00 O ATOM 953 CG2 THR A 69159.137 10.479 -0.146 1.00 0.00 C **ATOM** 954 H THR A 69160.967 7.138 -1.614 1.00 0.00 H **ATOM** 955 HA THR A 69161.399 9.091 0.486 1.00 0.00 H **ATOM** 956 HB THR A 69158.964 8.693 -1.259 1.00 0.00 H **ATOM** 957 HG1 THR A 69161.267 10.293 -1.655 1.00 0.00 H ATOM 958 1HG2 THR A 69158.646 11.126 -0.857 1.00 0.00 H **ATOM** 959 2HG2 THR A 69159.906 11.033 0.374 1.00 0.00 H **ATOM** 960 3HG2 THR A 69158.413 10.113 0.567 1.00 0.00 H **ATOM** 961 N ARGA 70160.389 7.706 2.306 1.00 0.00 N **ATOM** 962 CA ARG A 70159.699 7.084 3.429 1.00 0.00 C ATOM 963 C ARG A 70158.562 7.971 3.925 1.00 0.00 C ATOM 964 O ARG A 70158.773 9.132 4.275 1.00 0.00 O ATOM 965 CB ARG A 70160.680 6.807 4.569 1.00 0.00 C **ATOM** 966 CG ARG A 70160.151 5.828 5.603 1.00 0.00 C ATOM 967 CD ARG A 70160.885 5.964 6.927 1.00 0.00 C ATOM 968 NE ARG A 70162.332 5.847 6.766 1.00 0.00 N ATOM 969 CZ ARG A 70163.172 5.583 7.765 1.00 0.00 C **ATOM** 970 NH1 ARG A 70162.711 5.408 8.998 1.00 0.00 N **ATOM** 971 NH2 ARG A 70164.473 5.494 7.532 1.00 0.00 N **ATOM** 972 H ARG A 70161.285 8.080 2.443 1.00 0.00 H **ATOM** 973 HA ARG A 70159.286 6.147 3.086 1.00 0.00 H **ATOM** 974 1HB ARG A 70161.592 6.402 4.154 1.00 0.00 H **ATOM** 975 2HB ARG A 70160.906 7.738 5.069 1.00 0.00 H **ATOM** 976 1HG ARG A 70159.102 6.021 5.764 1.00 0.00 H **ATOM** 977 2HG ARG A 70160.282 4.821 5.232 1.00 0.00 H **ATOM** 978 1HD ARG A 70160.658 6.931 7.352 1.00 0.00 H **ATOM** 979 2HD ARG A 70160.543 5.189 7.596 1.00 0.00 H ATOM 980 HE ARG A 70162.699 5.971 5.866 1.00 0.00 H **ATOM** 981 1HH1 ARG A 70161.731 5.474 9.181 1.00 0.00 H ATOM

982 2HH1 ARG A 70163.347 5.210 9.744 1.00 0.00 H ATOM 983 1HH2 ARG A 70164.825 5.624 6.604 1.00 0.00 H **ATOM** 984 2HH2 ARG A 70165.104 5.296 8.282 1.00 0.00 H **ATOM** 985 N TYR A 71157.354 7.415 3.953 1.00 0.00 N **ATOM** 986 CA TYR A 71156.182 8.156 4.406 1.00 0.00 C **ATOM** 987 C TYR A 71155.796 7.749 5.824 1.00 0.00 C ATOM 988 O TYR A 71155.470 8.595 6.657 1.00 0.00 O ATOM 989 CB TYR A 71155.007 7.920 3.457 1.00 0.00 C **ATOM** 990 CG TYR A 71155.195 8.551 2.094 1.00 0.00 C ATOM 991 CD1 TYR A 71155.167 9.930 1.937 1.00 0.00 C ATOM 992 CD2 TYR A 71155.397 7.766 0.966 1.00 0.00 C ATOM 993 CE1 TYR A 71155.337 10.510 0.693 1.00 0.00 C **ATOM** 994 CE2 TYR A 71155.568 8.337 -0.280 1.00 0.00 C **ATOM** 995 CZ TYR A 71155.537 9.710 -0.411 1.00 0.00 C ATOM 996 OH TYR A 71155.707 10.284 -1.650 1.00 0.00 O **ATOM** 997 H TYR A 71157.249 6.486 3.661 1.00 0.00 H **ATOM** 998 HA TYR A 71156.432 9.207 4.401 1.00 0.00 H ATOM 999 1HB TYR A 71154.875 6.859 3.315 1.00 0.00 H ATOM ATOM 1000 2HB TYR A 71154.111 8.336 3.895 1.00 0.00 H ATOM 1001 HD1 TYR A 71155.010 10.555 2.804 1.00 0.00 H ATOM 1002 HD2 TYR A 71155.420 6.691 1.071 1.00 0.00 H ATOM 1003 HE1 TYR A 71155.313 11.585 0.592 1.00 0.00 H ATOM 1004 HE2 TYR A 71155.725 7.710 -1.145 1.00 0.00 H ATOM 1005 HH TYR A 71156.632 10.235 -1.902 1.00 0.00 H ATOM 1006 N PHE A 72155.835 6.447 6.092 1.00 0.00 N ATOM 1007 CA PHE A 72155.488 5.928 7.409 1.00 0.00 C ATOM 1008 C PHE A 72156.491 4.871 7.858 1.00 0.00 C ATOM 1009 O PHE A 72157.311 4.403 7.068 1.00 0.00 O ATOM 1010 CB PHE A 72154.079 5.335 7.393 1.00 0.00 C ATOM 1011 CG PHE A 72153.863 4.329 6.298 1.00 0.00 C ATOM 1012 CD1 PHE A 72154.015 2.974 6.546 1.00 0.00 C

ATOM 1013 CD2 PHE A 72153.508 4.738 5.023 1.00 0.00 C ATOM 1014 CE1 PHE A 72153.817 2.046 5.541 1.00 0.00 C ATOM 1015 CE2 PHE A 72153.309 3.816 4.015 1.00 0.00 C ATOM 1016 CZ PHE A 72153.463 2.468 4.274 1.00 0.00 C ATOM 1017 H PHE A 72156.102 5.823 5.386 1.00 0.00 H ATOM 1018 HA PHE A 72155.514 6.751 8.107 1.00 0.00 H ATOM 1019 1HB PHE A 72153.890 4.844 8.336 1.00 0.00 H ATOM 1020 2HB PHE A 72153.361 6.132 7.260 1.00 0.00 H ATOM 1021 HD1 PHE A 72154.290 2.644 7.537 1.00 0.00 H ATOM 1022 HD2 PHE A 72153.387 5.793 4.820 1.00 0.00 H ATOM 1023 HE1 PHE A 72153.939 0.993 5.746 1.00 0.00 H ATOM 1024 HE2 PHE A 72153.033 4.148 3.024 1.00 0.00 H ATOM 1025 HZ PHE A 72153.308 1.744 3.487 1.00 0.00 H ATOM 1026 N THR A 73156.422 4.500 9.133 1.00 0.00 N ATOM 1027 CA THR A 73157.326 3.498 9.688 1.00 0.00 C ATOM 1028 C THR A 73156.594 2.182 9.932 1.00 0.00 C ATOM 1029 O THR A 73155.767 2.079 10.838 1.00 0.00 O ATOM 1030 CB THR A 73157.941 4.003 10.993 1.00 0.00 C ATOM 1031 OG1 THR A 73156.941 4.531 11.848 1.00 0.00 O ATOM 1032 CG2 THR A 73158.983 5.080 10.785 1.00 0.00 C ATOM 1033 H THR A 73155.748 4.909 9.714 1.00 0.00 H ATOM 1034 HA THR A 73158.114 3.329 8.970 1.00 0.00 H ATOM 1035 HB THR A 73158.417 3.176 11.499 1.00 0.00 H ATOM 1036 HG1 THR A 73156.596 5.344 11.472 1.00 0.00 H ATOM 1037 1HG2 THR A 73159.375 5.392 11.742 1.00 0.00 H ATOM 1038 2HG2 THR A 73158.532 5.927 10.289 1.00 0.00 H ATOM 1039 3HG2 THR A 73159.786 4.692 10.177 1.00 0.00 H ATOM 1040 N CYS A 74156.905 1.178 9.118 1.00 0.00 N ATOM 1041 CA CYS A 74156.276 -0.132 9.247 1.00 0.00 C ATOM 1042 C CYS A 74157.327 -1.238 9.278 1.00 0.00 C ATOM 1043 O CYS A 74158.514 -0.986 9.073 1.00 0.00 O

ATOM 1044 CB CYS A 74155.305 -0.369 8.090 1.00 0.00 C ATOM 1045 SG CYS A 74153.619 0.197 8.415 1.00 0.00 S ATOM 1046 H CYS A 74157.572 1.322 8.415 1.00 0.00 H ATOM 1047 HA CYS A 74155.727 -0.147 10.176 1.00 0.00 H ATOM 1048 1HB CYS A 74155.662 0.153 7.215 1.00 0.00 H ATOM 1049 2HB CYS A 74155.261 -1.428 7.877 1.00 0.00 H ATOM 1050 HG CYS A 74153.098 0.048 7.623 1.00 0.00 H ATOM 1051 N ALAA 75156.880 -2.462 9.536 1.00 0.00 N ATOM 1052 CA ALAA 75157.781 -3.607 9.595 1.00 0.00 C ATOM 1053 C ALAA 75158.466 -3.836 8.251 1.00 0.00 C ATOM 1054 O ALAA 75158.120 -3.206 7.251 1.00 0.00 O ATOM 1055 CB ALAA 75157.022 -4.854 10.021 1.00 0.00 C ATOM 1056 H ALAA 75155.923 -2.600 9.691 1.00 0.00 H ATOM 1057 HA ALAA 75158.535 -3.401 10.341 1.00 0.00 H ATOM 1058 1HB ALA A 75156.775 -5.441 9.149 1.00 0.00 H ATOM 1059 2HB ALA A 75156.113 -4.566 10.529 1.00 0.00 H ATOM 1060 3HB ALA A 75157.636 -5.441 10.687 1.00 0.00 H ATOM 1061 N LEUA 76159.440 -4.741 8.235 1.00 0.00 N ATOM 1062 CA LEUA 76160.174 -5.052 7.014 1.00 0.00 C ATOM 1063 C LEU A 76159.372 -5.997 6.124 1.00 0.00 C ATOM 1064 O LEUA 76158.793 -6.973 6.600 1.00 0.00 O ATOM 1065 CB LEU A 76161.527 -5.679 7.353 1.00 0.00 C ATOM 1066 CG LEU A 76162.600 -4.692 7.818 1.00 0.00 C ATOM 1067 CD1 LEU A 76163.504 -5.337 8.856 1.00 0.00 C ATOM 1068 CD2 LEU A 76163.415 -4.197 6.633 1.00 0.00 C ATOM 1069 H LEUA 76159.671 -5.210 9.064 1.00 0.00 H ATOM 1070 HA LEU A 76160.339 -4.129 6.482 1.00 0.00 H ATOM 1071 1HB LEU A 76161.376 -6.410 8.135 1.00 0.00 H ATOM 1072 2HB LEU A 76161.895 -6.189 6.475 1.00 0.00 H ATOM 1073 HG LEU A 76162.121 -3.839 8.276 1.00 0.00 H ATOM 1074 1HD1 LEU A 76163.112 -5.145 9.844 1.00 0.00 H ATOM 1075 2HD1 LEU A 76164.497 -4.919 8.777 1.00 0.00 H ATOM 1076 3HD1 LEU A 76163.547 -6.401 8.686 1.00 0.00 H ATOM 1077 1HD2 LEU A 76163.394 -4.936 5.846 1.00 0.00 H ATOM 1078 2HD2 LEU A 76164.436 -4.028 6.943 1.00 0.00 H ATOM 1079 3HD2 LEU A 76162.993 -3.271 6.267 1.00 0.00 H ATOM 1080 N LYS A 77159.343 -5.699 4.829 1.00 0.00 N ATOM 1081 CA LYS A 77158.612 -6.522 3.872 1.00 0.00 C ATOM 1082 C LYS A 77157.123 -6.548 4.201 1.00 0.00 C ATOM 1083 O LYS A 77156.500 -7.610 4.224 1.00 0.00 O ATOM 1084 CB LYS A 77159.172 -7.946 3.859 1.00 0.00 C ATOM 1085 CG LYS A 77160.683 -8.006 3.706 1.00 0.00 C ATOM 1086 CD LYS A 77161.119 -7.581 2.314 1.00 0.00 C ATOM 1087 CE LYS A 77162.513 -6.976 2.326 1.00 0.00 C ATOM 1088 NZ LYS A 77163.560 -7.995 2.614 1.00 0.00 N ATOM 1089 H LYS A 77159.825 -4.908 4.510 1.00 0.00 H ATOM 1090 HA LYS A 77158.744 -6.086 2.892 1.00 0.00 H ATOM 1091 1HB LYS A 77158.907 -8.433 4.787 1.00 0.00 H ATOM 1092 2HB LYS A 77158.728 -8.489 3.038 1.00 0.00 H ATOM 1093 1HG LYS A 77161.135 -7.344 4.431 1.00 0.00 H ATOM 1094 2HG LYS A 77161.014 -9.018 3.886 1.00 0.00 H ATOM 1095 1HD LYS A 77161.120 -8.447 1.668 1.00 0.00 H ATOM 1096 2HD LYS A 77160.421 -6.849 1.936 1.00 0.00 H ATOM 1097 1HE LYS A 77162.708 -6.535 1.361 1.00 0.00 H ATOM 1098 2HE LYS A 77162.552 -6.209 3.086 1.00 0.00 H ATOM 1099 1HZ LYS A 77163.525 -8.270 3.616 1.00 0.00 H ATOM 1100 2HZ LYS A 77164.502 -7.610 2.403 1.00 0.00 H ATOM 1101 3HZ LYS A 77163.404 -8.841 2.028 1.00 0.00 H ATOM 1102 N LYS A 78156.558 -5.373 4.456 1.00 0.00 N ATOM 1103 CA LYS A 78155.142 -5.261 4.785 1.00 0.00 C ATOM 1104 C LYS A 78154.602 -3.885 4.407 1.00 0.00 C ATOM 1105 O LYS A 78153.781 -3.312 5.123 1.00 0.00 O

ATOM 1106 CB LYS A 78154.921 -5.517 6.278 1.00 0.00 C ATOM 1107 CG LYS A 78155.477 -6.850 6.755 1.00 0.00 C ATOM 1108 CD LYS A 78155.149 -7.097 8.218 1.00 0.00 C ATOM 1109 CE LYS A 78153.954 -8.023 8.373 1.00 0.00 C ATOM 1110 NZ LYS A 78153.139 -7.684 9.573 1.00 0.00 N ATOM 1111 H LYS A 78157.106 -4.561 4.423 1.00 0.00 H ATOM 1112 HA LYS A 78154.610 -6.012 4.219 1.00 0.00 H ATOM 1113 1HB LYS A 78155.400 -4.729 6.840 1.00 0.00 H ATOM 1114 2HB LYS A 78153.861 -5.500 6.482 1.00 0.00 H ATOM 1115 1HG LYS A 78155.046 -7.641 6.161 1.00 0.00 H ATOM 1116 2HG LYS A 78156.550 -6.845 6.631 1.00 0.00 H ATOM 1117 1HD LYS A 78156.005 -7.550 8.697 1.00 0.00 H ATOM 1118 2HD LYS A 78154.926 -6.152 8.692 1.00 0.00 H ATOM 1119 1HE LYS A 78153.332 -7.938 7.493 1.00 0.00 H ATOM 1120 2HE LYS A 78154.309 -9.038 8.464 1.00 0.00 H ATOM 1121 1HZ LYS A 78152.325 -8.326 9.645 1.00 0.00 H ATOM 1122 2HZ LYS A 78152.792 -6.707 9.505 1.00 0.00 H ATOM 1123 3HZ LYS A 78153.716 -7.775 10.433 1.00 0.00 H ATOM 1124 N ALAA 79155.068 -3.363 3.278 1.00 0.00 N ATOM 1125 CA ALAA 79154.633 -2.055 2.805 1.00 0.00 C ATOM 1126 C ALA A 79154.555 -2.020 1.282 1.00 0.00 C ATOM 1127 O ALAA 79155.578 -1.989 0.599 1.00 0.00 O ATOM 1128 CB ALA A 79155.571 -0.971 3.312 1.00 0.00 C ATOM 1129 H ALA A 79155.721 -3.869 2.751 1.00 0.00 H ATOM 1130 HA ALAA 79153.648 -1.864 3.209 1.00 0.00 H ATOM 1131 1HB ALA A 79156.010 -1.283 4.248 1.00 0.00 H ATOM 1132 2HB ALA A 79155.017 -0.056 3.462 1.00 0.00 H ATOM 1133 3HB ALA A 79156.353 -0.802 2.586 1.00 0.00 H ATOM 1134 N LEUA 80153.334 -2.025 0.757 1.00 0.00 N ATOM 1135 CA LEU A 80153.122 -1.994 -0.685 1.00 0.00 C ATOM 1136 C LEUA 80152.248 -0.809 -1.081 1.00 0.00 C

ATOM 1137 O LEUA 80151.047 -0.791 -0.810 1.00 0.00 O ATOM 1138 CB LEU A 80152.476 -3.299 -1.154 1.00 0.00 C ATOM 1139 CG LEU A 80152.145 -3.358 -2.647 1.00 0.00 C ATOM 1140 CD1 LEU A 80153.393 -3.669 -3.458 1.00 0.00 C ATOM 1141 CD2 LEU A 80151.062 -4.394 -2.911 1.00 0.00 C ATOM 1142 H LEU A 80152.557 -2.050 1.353 1.00 0.00 H ATOM 1143 HA LEU A 80154.086 -1.889 -1.160 1.00 0.00 H ATOM 1144 1HB LEU A 80153.147 -4.113 -0.923 1.00 0.00 H ATOM 1145 2HB LEU A 80151.559 -3.442 -0.600 1.00 0.00 H ATOM 1146 HG LEU A 80151.772 -2.395 -2.964 1.00 0.00 H ATOM 1147 1HD1 LEU A 80153.335 -3.169 -4.413 1.00 0.00 H ATOM 1148 2HD1 LEU A 80153.464 -4.735 -3.614 1.00 0.00 H ATOM 1149 3HD1 LEU A 80154.265 -3.325 -2.923 1.00 0.00 H ATOM 1150 1HD2 LEU A 80150.263 -4.270 -2.196 1.00 0.00 H ATOM 1151 2HD2 LEU A 80151.481 -5.385 -2.814 1.00 0.00 H ATOM 1152 3HD2 LEU A 80150.675 -4.263 -3.911 1.00 0.00 H ATOM 1153 N PHE A 81152.858 0.182 -1.724 1.00 0.00 N ATOM 1154 CA PHE A 81152.135 1.371 -2.158 1.00 0.00 C ATOM 1155 C PHE A 81151.374 1.103 -3.452 1.00 0.00 C ATOM 1156 O PHE A 81151.879 0.436 -4.355 1.00 0.00 O ATOM 1157 CB PHE A 81153.104 2.538 -2.355 1.00 0.00 C ATOM 1158 CG PHE A 81153.883 2.888 -1.119 1.00 0.00 C ATOM 1159 CD1 PHE A 81153.494 3.947 -0.316 1.00 0.00 C ATOM 1160 CD2 PHE A 81155.005 2.157 -0.761 1.00 0.00 C ATOM 1161 CE1 PHE A 81154.209 4.271 0.822 1.00 0.00 C ATOM 1162 CE2 PHE A 81155.724 2.476 0.375 1.00 0.00 C ATOM 1163 CZ PHE A 81155.325 3.534 1.167 1.00 0.00 C ATOM 1164 H PHE A 81153.817 0.110 -1.911 1.00 0.00 H ATOM 1165 HA PHE A 81151.428 1.630 -1.385 1.00 0.00 H ATOM 1166 1HB PHE A 81153.810 2.283 -3.131 1.00 0.00 H ATOM 1167 2HB PHE A 81152.546 3.414 -2.656 1.00 0.00 H

ATOM 1168 HD1 PHE A 81152.621 4.524 -0.585 1.00 0.00 H ATOM 1169 HD2 PHE A 81155.317 1.329 -1.381 1.00 0.00 H ATOM 1170 HE1 PHE A 81153.895 5.100 1.440 1.00 0.00 H ATOM 1171 HE2 PHE A 81156.596 1.898 0.643 1.00 0.00 H ATOM 1172 HZ PHE A 81155.884 3.785 2.056 1.00 0.00 H ATOM 1173 N VALA 82150.155 1.628 -3.535 1.00 0.00 N ATOM 1174 CA VALA 82149.324 1.445 -4.718 1.00 0.00 C ATOM 1175 C VALA 82148.369 2.618 -4.907 1.00 0.00 C ATOM 1176 O VALA 82148.190 3.437 -4.005 1.00 0.00 O ATOM 1177 CB VALA 82148.507 0.142 -4.635 1.00 0.00 C ATOM 1178 CG1 VAL A 82149.423 -1.069 -4.717 1.00 0.00 C ATOM 1179 CG2 VAL A 82147.682 0.111 -3.358 1.00 0.00 C ATOM 1180 H VALA 82149.807 2.151 -2.782 1.00 0.00 H ATOM 1181 HA VALA 82149.976 1.382 -5.577 1.00 0.00 H ATOM 1182 HB VALA 82147.830 0.111 -5.477 1.00 0.00 H ATOM 1183 1HG1 VAL A 82150.197 -0.886 -5.447 1.00 0.00 H ATOM 1184 2HG1 VAL A 82148.848 -1.936 -5.010 1.00 0.00 H ATOM 1185 3HG1 VAL A 82149.873 -1.247 -3.751 1.00 0.00 H ATOM 1186 1HG2 VAL A 82147.413 1.118 -3.078 1.00 0.00 H ATOM 1187 2HG2 VAL A 82148.261 -0.341 -2.566 1.00 0.00 H ATOM 1188 3HG2 VAL A 82146.784 -0.468 -3.523 1.00 0.00 H ATOM 1189 N LYS A 83147.757 2.694 -6.084 1.00 0.00 N ATOM 1190 CA LYS A 83146.820 3.768 -6.391 1.00 0.00 C ATOM 1191 C LYS A 83145.576 3.672 -5.515 1.00 0.00 C ATOM 1192 O LYS A 83144.875 2.659 -5.521 1.00 0.00 O ATOM 1193 CB LYS A 83146.424 3.721 -7.868 1.00 0.00 C ATOM 1194 CG LYS A 83147.590 3.945 -8.818 1.00 0.00 C ATOM 1195 CD LYS A 83147.222 3.577 -10.246 1.00 0.00 C ATOM 1196 CE LYS A 83147.832 4.546 -11.246 1.00 0.00 C ATOM 1197 NZ LYS A 83148.273 3.859 -12.490 1.00 0.00 N ATOM 1198 H LYS A 83147.941 2.011 -6.763 1.00 0.00 H

ATOM 1199 HA LYS A 83147.313 4.707 -6.190 1.00 0.00 H ATOM 1200 1HB LYS A 83145.993 2.754 -8.081 1.00 0.00 H ATOM 1201 2HB LYS A 83145.684 4.484 -8.054 1.00 0.00 H ATOM 1202 1HG LYS A 83147.871 4.986 -8.786 1.00 0.00 H ATOM 1203 2HG LYS A 83148.421 3.334 -8.500 1.00 0.00 H ATOM 1204 1HD LYS A 83147.587 2.583 -10.456 1.00 0.00 H ATOM 1205 2HD LYS A 83146.147 3.598 -10.349 1.00 0.00 H ATOM 1206 1HE LYS A 83147.095 5.293 -11.500 1.00 0.00 H ATOM 1207 2HE LYS A 83148.686 5.025 -10.788 1.00 0.00 H ATOM 1208 1HZ LYS A 83149.279 3.605 -12.422 1.00 0.00 H ATOM 1209 2HZ LYS A 83148.139 4.483 -13.310 1.00 0.00 H ATOM 1210 3HZ LYS A 83147.717 2.991 -12.635 1.00 0.00 H ATOM 1211 N LEU A 84145.307 4.735 -4.765 1.00 0.00 N ATOM 1212 CA LEU A 84144.147 4.776 -3.883 1.00 0.00 C ATOM 1213 C LEU A 84142.855 4.587 -4.673 1.00 0.00 C ATOM 1214 O LEU A 84141.893 4.002 -4.176 1.00 0.00 O ATOM 1215 CB LEU A 84144.108 6.105 -3.127 1.00 0.00 C ATOM 1216 CG LEU A 84142.878 6.316 -2.242 1.00 0.00 C ATOM 1217 CD1 LEU A 84143.016 5.538 -0.942 1.00 0.00 C ATOM 1218 CD2 LEU A 84142.672 7.795 -1.961 1.00 0.00 C ATOM 1219 H LEU A 84145.903 5.510 -4.806 1.00 0.00 H ATOM 1220 HA LEU A 84144.242 3.970 -3.172 1.00 0.00 H ATOM 1221 1HB LEU A 84144.989 6.165 -2.504 1.00 0.00 H ATOM 1222 2HB LEU A 84144.145 6.906 -3.849 1.00 0.00 H ATOM 1223 HG LEU A 84142.004 5.947 -2.760 1.00 0.00 H ATOM 1224 1HD1 LEU A 84142.131 5.683 -0.340 1.00 0.00 H ATOM 1225 2HD1 LEU A 84143.882 5.890 -0.401 1.00 0.00 H ATOM 1226 3HD1 LEU A 84143.134 4.486 -1.162 1.00 0.00 H ATOM 1227 1HD2 LEU A 84141.827 7.923 -1.300 1.00 0.00 H ATOM 1228 2HD2 LEU A 84142.485 8.316 -2.887 1.00 0.00 H ATOM 1229 3HD2 LEU A 84143.558 8.200 -1.493 1.00 0.00 H ATOM 1230 N LYS A 85142.843 5.085 -5.904 1.00 0.00 N ATOM 1231 CA LYS A 85141.670 4.971 -6.764 1.00 0.00 C ATOM 1232 C LYS A 85141.371 3.510 -7.086 1.00 0.00 C ATOM 1233 O LYS A 85140.226 3.147 -7.355 1.00 0.00 O ATOM 1234 CB LYS A 85141.882 5.757 -8.059 1.00 0.00 C ATOM 1235 CG LYS A 85143.234 5.509 -8.708 1.00 0.00 C ATOM 1236 CD LYS A 85144.209 6.639 -8.416 1.00 0.00 C ATOM 1237 CE LYS A 85145.050 6.980 -9.635 1.00 0.00 C ATOM 1238 NZ LYS A 85145.823 8.237 -9.443 1.00 0.00 N ATOM 1239 H LYS A 85143.642 5.540 -6.244 1.00 0.00 H ATOM 1240 HA LYS A 85140.829 5.389 -6.232 1.00 0.00 H ATOM 1241 1HB LYS A 85141.112 5.481 -8.764 1.00 0.00 H ATOM 1242 2HB LYS A 85141.798 6.812 -7.842 1.00 0.00 H ATOM 1243 1HG LYS A 85143.642 4.587 -8.325 1.00 0.00 H ATOM 1244 2HG LYS A 85143.099 5.429 -9.776 1.00 0.00 H ATOM 1245 1HD LYS A 85143.653 7.515 -8.119 1.00 0.00 H ATOM 1246 2HD LYS A 85144.863 6.336 -7.611 1.00 0.00 H ATOM 1247 1HE LYS A 85145,739 6,169 -9,820 1,00 0,00 H ATOM 1248 2HE LYS A 85144.396 7.096 -10.487 1.00 0.00 H ATOM 1249 1HZ LYS A 85145.341 8.853 -8.758 1.00 0.00 H ATOM 1250 2HZ LYS A 85145.911 8.745 -10.346 1.00 0.00 H ATOM 1251 3HZ LYS A 85146.777 8.020 -9.087 1.00 0.00 H ATOM 1252 N SER A 86142.405 2.675 -7.058 1.00 0.00 N ATOM 1253 CA SER A 86142.248 1.255 -7.348 1.00 0.00 C ATOM 1254 C SER A 86142.150 0.442 -6.061 1.00 0.00 C ATOM 1255 O SER A 86142.547 -0.722 -6.017 1.00 0.00 O ATOM 1256 CB SER A 86143.421 0.752 -8.193 1.00 0.00 C ATOM 1257 OG SER A 86143,705 1.648 -9.254 1.00 0.00 O ATOM 1258 H SER A 86143.295 3.023 -6.838 1.00 0.00 H ATOM 1259 HA SER A 86141.334 1.130 -7.908 1.00 0.00 H ATOM 1260 1HB SER A 86144.298 0.663 -7.569 1.00 0.00 H ATOM 1261 2HB SER A 86143.176 -0.214 -8.608 1.00 0.00 H ATOM 1262 HG SER A 86144.344 1.247 -9.848 1.00 0.00 H ATOM 1263 N CYS A 87141.618 1.064 -5.012 1.00 0.00 N ATOM 1264 CA CYS A 87141.467 0.398 -3.724 1.00 0.00 C ATOM 1265 C CYS A 87139.994 0.260 -3.353 1.00 0.00 C ATOM 1266 O CYS A 87139.165 1.081 -3.747 1.00 0.00 O ATOM 1267 CB CYS A 87142.207 1.175 -2.634 1.00 0.00 C ATOM 1268 SG CYS A 87143.989 0.867 -2.590 1.00 0.00 S ATOM 1269 H CYS A 87141.319 1.992 -5.108 1.00 0.00 H ATOM 1270 HA CYS A 87141.898 -0.588 -3.808 1.00 0.00 H ATOM 1271 1HB CYS A 87142.062 2.233 -2.795 1.00 0.00 H ATOM 1272 2HB CYS A 87141.802 0.904 -1.670 1.00 0.00 H ATOM 1273 HG CYS A 87144.418 1.539 -3.125 1.00 0.00 H ATOM 1274 N ARG A 88139.674 -0.783 -2.595 1.00 0.00 N ATOM 1275 CA ARG A 88138.300 -1.027 -2.172 1.00 0.00 C ATOM 1276 C ARG A 88138.226 -1.247 -0.662 1.00 0.00 C ATOM 1277 O ARG A 88139.134 -1.828 -0.067 1.00 0.00 O ATOM 1278 CB ARG A 88137.728 -2.243 -2.903 1.00 0.00 C ATOM 1279 CG ARG A 88137.135 -1.911 -4.264 1.00 0.00 C ATOM 1280 CD ARG A 88135.620 -1.785 -4.199 1.00 0.00 C ATOM 1281 NE ARG A 88135.175 -0.413 -4.428 1.00 0.00 N ATOM 1282 CZ ARG A 88135.192 0.183 -5.618 1.00 0.00 C ATOM 1283 NH1 ARG A 88135.631 -0.468 -6.688 1.00 0.00 N ATOM 1284 NH2 ARG A 88134.768 1.433 -5.740 1.00 0.00 N ATOM 1285 H ARG A 88140.378 -1.403 -2.312 1.00 0.00 H ATOM 1286 HA ARG A 88137.715 -0.156 -2.427 1.00 0.00 H ATOM 1287 1HB ARG A 88138.517 -2.967 -3.046 1.00 0.00 H ATOM 1288 2HB ARG A 88136.953 -2.684 -2.294 1.00 0.00 H ATOM 1289 1HG ARG A 88137.549 -0.974 -4.607 1.00 0.00 H ATOM 1290 2HG ARG A 88137.392 -2.697 -4.958 1.00 0.00 H ATOM 1291 1HD ARG A 88135.186 -2.424 -4.953 1.00 0.00 H ATOM 1292 2HD ARG A 88135.285 -2.103 -3.222 1.00 0.00 H ATOM 1293 HE ARG A 88134.846 0.092 -3.655 1.00 0.00 H ATOM 1294 1HH1 ARG A 88135.952 -1.412 -6.603 1.00 0.00 H ATOM 1295 2HH1 ARG A 88135.640 -0.016 -7.580 1.00 0.00 H ATOM 1296 1HH2 ARG A 88134.436 1.929 -4.938 1.00 0.00 H ATOM 1297 2HH2 ARG A 88134.780 1.881 -6.634 1.00 0.00 H ATOM 1298 N PRO A 89137.138 -0.787 -0.019 1.00 0.00 N ATOM 1299 CA PRO A 89136.954 -0.940 1.428 1.00 0.00 C ATOM 1300 C PRO A 89137.091 -2.390 1.877 1.00 0.00 C ATOM 1301 O PRO A 89136.444 -3.284 1.330 1.00 0.00 O ATOM 1302 CB PRO A 89135.526 -0.441 1.664 1.00 0.00 C ATOM 1303 CG PRO A 89135.249 0.476 0.523 1.00 0.00 C ATOM 1304 CD PRO A 89136.005 -0.084 -0.649 1.00 0.00 C ATOM 1305 HA PRO A 89137.650 -0.326 1.981 1.00 0.00 H ATOM 1306 1HB PRO A 89134.846 -1.280 1.672 1.00 0.00 H ATOM 1307 2HB PRO A 89135.476 0.079 2.609 1.00 0.00 H ATOM 1308 1HG PRO A 89134.189 0.491 0.314 1.00 0.00 H ATOM 1309 2HG PRO A 89135.602 1.469 0.758 1.00 0.00 H ATOM 1310 1HD PRO A 89135.384 -0.771 -1.205 1.00 0.00 H ATOM 1311 2HD PRO A 89136.354 0.714 -1.288 1.00 0.00 H ATOM 1312 N ASPA 90137.937 -2.618 2.876 1.00 0.00 N ATOM 1313 CA ASPA 90138.157 -3.961 3.398 1.00 0.00 C ATOM 1314 C ASPA 90137.366 -4.181 4.683 1.00 0.00 C ATOM 1315 O ASPA 90137.759 -3.716 5.754 1.00 0.00 O ATOM 1316 CB ASP A 90139.647 -4.192 3.658 1.00 0.00 C ATOM 1317 CG ASPA 90140.036 -5.653 3.537 1.00 0.00 C ATOM 1318 OD1 ASP A 90140.335 -6.275 4.578 1.00 0.00 O ATOM 1319 OD2 ASP A 90140.041 -6.174 2.403 1.00 0.00 O ATOM 1320 H ASPA 90138.424 -1.866 3.271 1.00 0.00 H ATOM 1321 HA ASPA 90137.817 -4.667 2.655 1.00 0.00 H ATOM 1322 1HB ASP A 90140.223 -3.626 2.941 1.00 0.00 H

ATOM 1323 2HB ASP A 90139.889 -3.855 4.654 1.00 0.00 H ATOM 1324 N SER A 91136.249 -4.893 4.571 1.00 0.00 N ATOM 1325 CA SER A 91135.403 -5.173 5.725 1.00 0.00 C ATOM 1326 C SER A 91135.694 -6.560 6.292 1.00 0.00 C ATOM 1327 O SER A 91134.834 -7.177 6.920 1.00 0.00 O ATOM 1328 CB SER A 91133.928 -5.070 5.339 1.00 0.00 C ATOM 1329 OG SER A 91133.139 -4.656 6.440 1.00 0.00 O ATOM 1330 H SER A 91135.988 -5.237 3.691 1.00 0.00 H ATOM 1331 HA SER A 91135.620 -4.435 6.482 1.00 0.00 H ATOM 1332 1HB SER A 91133.815 -4.351 4.541 1.00 0.00 H ATOM 1333 2HB SER A 91133.577 -6.036 5.005 1.00 0.00 H ATOM 1334 HG SER A 91132.431 -5.288 6.584 1.00 0.00 H ATOM 1335 N ARG A 92136.912 -7.045 6.069 1.00 0.00 N ATOM 1336 CA ARG A 92137.312 -8.358 6.561 1.00 0.00 C ATOM 1337 C ARG A 92137.327 -8.385 8.086 1.00 0.00 C ATOM 1338 O ARG A 92137.097 -9.426 8.702 1.00 0.00 O ATOM 1339 CB ARG A 92138.693 -8.731, 6.019 1.00 0.00 C ATOM 1340 CG ARG A 92138.670 -9.221 4.580 1.00 0.00 C ATOM 1341 CD ARG A 92137.825 -10.475 4.432 1.00 0.00 C ATOM 1342 NE ARG A 92136.492 -10.179 3.911 1.00 0.00 N ATOM 1343 CZ ARG A 92136.232 -9.956 2.624 1.00 0.00 C ATOM 1344 NH1 ARG A 92137.209 -9.994 1.726 1.00 0.00 N ATOM 1345 NH2 ARG A 92134.992 -9.695 2.235 1.00 0.00 N ATOM 1346 H ARG A 92137.557 -6.509 5.564 1.00 0.00 H ATOM 1347 HA ARG A 92136.589 -9.078 6.208 1.00 0.00 H ATOM 1348 1HB ARG A 92139.334 -7.863 6.072 1.00 0.00 H ATOM 1349 2HB ARG A 92139.110 -9.513 6.636 1.00 0.00 H ATOM 1350 1HG ARG A 92138.257 -8.444 3.953 1.00 0.00 H ATOM 1351 2HG ARG A 92139.681 -9.438 4.269 1.00 0.00 H ATOM 1352 1HD ARG A 92138.324 -11.152 3.755 1.00 0.00 H ATOM 1353 2HD ARG A 92137.726 -10.944 5.400 1.00 0.00 H ATOM 1354 HE ARG A 92135.752 -10.145 4.552 1.00 0.00 H ATOM 1355 1HH1 ARG A 92138.147 -10.191 2.013 1.00 0.00 H ATOM 1356 2HH1 ARG A 92137.007 -9.826 0.761 1.00 0.00 H ATOM 1357 1HH2 ARG A 92134.252 -9.666 2.907 1.00 0.00 H ATOM 1358 2HH2 ARG A 92134.796 -9.528 1.268 1.00 0.00 H ATOM 1359 N PHE A 93137.598 -7.232 8.690 1.00 0.00 N ATOM 1360 CA PHE A 93137.643 -7.121 10.144 1.00 0.00 C ATOM 1361 C PHE A 93136.506 -6.246 10.661 1.00 0.00 C ATOM 1362 O PHE A 93136.622 -5.622 11.715 1.00 0.00 O ATOM 1363 CB PHE A 93138.988 -6.547 10.591 1.00 0.00 C ATOM 1364 CG PHE A 93140.161 -7.413 10.229 1.00 0.00 C ATOM 1365 CD1 PHE A 93140.944 -7.988 11.217 1.00 0.00 C ATOM 1366 CD2 PHE A 93140.480 -7.652 8.903 1.00 0.00 C ATOM 1367 CE1 PHE A 93142.023 -8.787 10.889 1.00 0.00 C ATOM 1368 CE2 PHE A 93141.558 -8.449 8.567 1.00 0.00 C ATOM 1369 CZ PHE A 93142.331 -9.016 9.562 1.00 0.00 C ATOM 1370 H PHE A 93137.773 -6.436 8.146 1.00 0.00 H ATOM 1371 HA PHE A 93137.532 -8.114 10.555 1.00 0.00 H ATOM 1372 1HB PHE A 93139.132 -5.582 10.125 1.00 0.00 H ATOM 1373 2HB PHE A 93138.981 -6.425 11.664 1.00 0.00 H ATOM 1374 HD1 PHE A 93140.704 -7.809 12.255 1.00 0.00 H ATOM 1375 HD2 PHE A 93139.877 -7.208 8.124 1.00 0.00 H ATOM 1376 HE1 PHE A 93142.625 -9.228 11.668 1.00 0.00 H ATOM 1377 HE2 PHE A 93141.797 -8.627 7.529 1.00 0.00 H ATOM 1378 HZ PHE A 93143.175 -9.640 9.302 1.00 0.00 H ATOM 1379 N ALAA 94135.407 -6.203 9.912 1.00 0.00 N ATOM 1380 CA ALA A 94134.252 -5.403 10.300 1.00 0.00 C ATOM 1381 C ALA A 94133.515 -6.036 11.474 1.00 0.00 C ATOM 1382 O ALAA 94133.186 -7.221 11.448 1.00 0.00 O ATOM 1383 CB ALA A 94133.311 -5.227 9.116 1.00 0.00 C ATOM 1384 H ALAA 94135.373 -6.721 9.081 1.00 0.00 H

ATOM 1385 HA ALAA 94134.607 -4.426 10.594 1.00 0.00 H ATOM 1386 1HB ALAA 94133.533 -4.295 8.616 1.00 0.00 H ATOM 1387 2HB ALA A 94132.291 -5.213 9.466 1.00 0.00 H ATOM 1388 3HB ALA A 94133.444 -6.047 8.426 1.00 0.00 H ATOM 1389 N SER A 95133.257 -5.236 12.504 1.00 0.00 N ATOM 1390 CA SER A 95132.557 -5.717 13.689 1.00 0.00 C ATOM 1391 C SER A 95131.078 -5.939 13.396 1.00 0.00 C ATOM 1392 O SER A 95130.347 -4.997 13.093 1.00 0.00 O ATOM 1393 CB SER A 95132.718 -4.723 14.840 1.00 0.00 C ATOM 1394 OG SER A 95134.071 -4.626 15.247 1.00 0.00 O ATOM 1395 H SER A 95133.544 -4.299 12.466 1.00 0.00 H ATOM 1396 HA SER A 95133.001 -6.659 13.975 1.00 0.00 H ATOM 1397 1HB SER A 95132.379 -3.748 14.522 1.00 0.00 H ATOM 1398 2HB SER A 95132.124 -5.052 15.682 1.00 0.00 H ATOM 1399 HG SER A 95134.111 -4.383 16.175 1.00 0.00 H ATOM 1400 N LEUA 96130.643 -7.192 13.488 1.00 0.00 N ATOM 1401 CA LEU A 96129.250 -7.537 13.233 1.00 0.00 C ATOM 1402 C LEUA 96128.828 -8.744 14.064 1.00 0.00 C ATOM 1403 O LEUA 96128.824 -9.876 13.579 1.00 0.00 O ATOM 1404 CB LEU A 96129.039 -7.830 11.746 1.00 0.00 C ATOM 1405 CG LEU A 96128.713 -6.609 10.885 1.00 0.00 C ATOM 1406 CD1 LEU A 96129.040 -6.881 9.425 1.00 0.00 C ATOM 1407 CD2 LEU A 96127.249 -6.224 11.042 1.00 0.00 C ATOM 1408 H LEUA 96131.274 -7.900 13.734 1.00 0.00 H ATOM 1409 HA LEU A 96128.642 -6.691 13.513 1.00 0.00 H ATOM 1410 1HB LEU A 96129.940 -8.286 11.359 1.00 0.00 H ATOM 1411 2HB LEU A 96128.229 -8.537 11.650 1.00 0.00 H ATOM 1412 HG LEU A 96129.316 -5.774 11.212 1.00 0.00 H ATOM 1413 1HD1 LEU A 96129.355 -5.964 8.950 1.00 0.00 H ATOM 1414 2HD1 LEU A 96128.163 -7.263 8.924 1.00 0.00 H ATOM 1415 3HD1 LEU A 96129.835 -7.609 9.364 1.00 0.00 H ATOM 1416 1HD2 LEU A 96126.884 -5.810 10.114 1.00 0.00 H ATOM 1417 2HD2 LEU A 96127.153 -5.488 11.828 1.00 0.00 H ATOM 1418 3HD2 LEU A 96126.672 -7.100 11.298 1.00 0.00 H ATOM 1419 N GLN A 97128.471 -8.495 15.320 1.00 0.00 N ATOM 1420 CA GLN A 97128.046 -9.560 16.220 1.00 0.00 C ATOM 1421 C GLN A 97126.659 -9.272 16.790 1.00 0.00 C ATOM 1422 O GLN A 97126.264 -8.114 16.928 1.00 0.00 O ATOM 1423 CB GLN A 97129.053 -9.725 17.361 1.00 0.00 C ATOM 1424 CG GLN A 97130.174 -10.704 17.045 1.00 0.00 C ATOM 1425 CD GLN A 97130.874 -11.208 18.292 1.00 0.00 C ATOM 1426 OE1 GLN A 97130.231 -11.632 19.251 1.00 0.00 O ATOM 1427 NE2 GLN A 97132.201 -11.162 18.283 1.00 0.00 N ATOM 1428 H GLN A 97128.494 -7.572 15.649 1.00 0.00 H ATOM 1429 HA GLN A 97128.005 -10.478 15.653 1.00 0.00 H ATOM 1430 1HB GLN A 97129.495 -8.764 17.578 1.00 0.00 H ATOM 1431 2HB GLN A 97128.533 -10.079 18.238 1.00 0.00 H ATOM 1432 1HG GLN A 97129.758 -11.550 16.518 1.00 0.00 H ATOM 1433 2HG GLN A 97130.899 -10.209 16.417 1.00 0.00 H ATOM 1434 1HE2 GLN A 97132.647 -10.812 17.485 1.00 0.00 H ATOM 1435 2HE2 GLN A 97132.681 -11.482 19.076 1.00 0.00 H ATOM 1436 N PRO A 98125.898 -10.327 17.129 1.00 0.00 N ATOM 1437 CA PRO A 98124.549 -10.181 17.686 1.00 0.00 C ATOM 1438 C PRO A 98124.566 -9.615 19.102 1.00 0.00 C ATOM 1439 O PRO A 98125.628 -9.439 19.699 1.00 0.00 O ATOM 1440 CB PRO A 98124.009 -11.613 17.690 1.00 0.00 C ATOM 1441 CG PRO A 98125.221 -12.475 17.756 1.00 0.00 C ATOM 1442 CD PRO A 98126.294 -11.743 16.998 1.00 0.00 C ATOM 1443 HA PRO A 98123.928 -9.560 17.059 1.00 0.00 H ATOM 1444 1HB PRO A 98123.372 -11.758 18.549 1.00 0.00 H ATOM 1445 2HB PRO A 98123.448 -11.791 16.784 1.00 0.00 H ATOM 1446 1HG PRO A 98125.517 -12.613 18.785 1.00 0.00 H

ATOM 1447 2HG PRO A 98125.019 -13.429 17.291 1.00 0.00 H ATOM 1448 1HD PRO A 98127.259 -11.917 17.448 1.00 0.00 H ATOM 1449 2HD PRO A 98126.297 -12.046 15.962 1.00 0.00 H ATOM 1450 N SER A 99123.382 -9.331 19.634 1.00 0.00 N ATOM 1451 CA SER A 99123.259 -8.784 20.981 1.00 0.00 C ATOM 1452 C SER A 99122.426 -9.703 21.868 1.00 0.00 C ATOM 1453 O SER A 99121.262 -9.977 21.575 1.00 0.00 O ATOM 1454 CB SER A 99122.626 -7.392 20.932 1.00 0.00 C ATOM 1455 OG SER A 99123.485 -6.463 20.292 1.00 0.00 O ATOM 1456 H SER A 99122.570 -9.493 19.109 1.00 0.00 H ATOM 1457 HA SER A 99124.252 -8.704 21.398 1.00 0.00 H ATOM 1458 1HB SER A 99121.697 -7.440 20.385 1.00 0.00 H ATOM 1459 2HB SER A 99122.434 -7.051 21.939 1.00 0.00 H ATOM 1460 HG SER A 99123.508 -5.648 20.798 1.00 0.00 H ATOM 1461 N GLY A 100123.030 -10.177 22.953 1.00 0.00 N ATOM 1462 CA GLY A 100122.328 -11.060 23.866 1.00 0.00 C ATOM 1463 C GLY A 100123.264 -11.750 24.840 1.00 0.00 C ATOM 1464 O GLY A 100124.480 -11.744 24.645 1.00 0.00 O ATOM 1465 H GLY A 100123.958 -9.925 23.135 1.00 0.00 H ATOM 1466 1HA GLY A 100121.606 -10.483 24.424 1.00 0.00 H ATOM 1467 2HA GLY A 100121.806 -11.811 23.292 1.00 0.00 H ATOM 1468 N PRO A 101122.723 -12.361 25.909 1.00 0.00 N ATOM 1469 CA PRO A 101123.532 -13.058 26.914 1.00 0.00 C ATOM 1470 C PRO A 101124.481 -14.075 26.289 1.00 0.00 C ATOM 1471 O PRO A 101124.058 -15.142 25.844 1.00 0.00 O ATOM 1472 CB PRO A 101122.490 -13.764 27.784 1.00 0.00 C ATOM 1473 CG PRO A 101121.251 -12.951 27.626 1.00 0.00 C ATOM 1474 CD PRO A 101121.283 -12.419 26.220 1.00 0.00 C ATOM 1475 HA PRO A 101124.098 -12.363 27.517 1.00 0.00 H ATOM 1476 1HB PRO A 101122.347 -14.775 27.430 1.00 0.00 H ATOM 1477 2HB PRO A 101122.824 -13.779 28.810 1.00 0.00 H ATOM 1478 1HG PRO A 101120.382 -13.575 27.772 1.00 0.00 H ATOM 1479 2HG PRO A 101121.254 -12.137 28.336 1.00 0.00 H ATOM 1480 1HD PRO A 101120.770 -13.092 25.550 1.00 0.00 H ATOM 1481 2HD PRO A 101120.841 -11.434 26.180 1.00 0.00 H ATOM 1482 N SER A 102125.766 -13.737 26.259 1.00 0.00 N ATOM 1483 CA SER A 102126.776 -14.621 25.688 1.00 0.00 C ATOM 1484 C SER A 102128.162 -14.283 26.226 1.00 0.00 C ATOM 1485 O SER A 102128.405 -13.168 26.686 1.00 0.00 O ATOM 1486 CB SER A 102126.769 -14.520 24.162 1.00 0.00 C ATOM 1487 OG SER A 102127.881 -15.196 23.599 1.00 0.00 O ATOM 1488 H SER A 102126.042 -12.874 26.629 1.00 0.00 H ATOM 1489 HA SER A 102126.528 -15.633 25.973 1.00 0.00 H ATOM 1490 1HB SER A 102125.863 -14.962 23.776 1.00 0.00 H ATOM 1491 2HB SER A 102126.812 -13.480 23.873 1.00 0.00 H ATOM 1492 HG SER A 102128.175 -14.731 22.813 1.00 0.00 H ATOM 1493 N SER A 103129.067 -15.254 26.164 1.00 0.00 N ATOM 1494 CA SER A 103130.431 -15.060 26.645 1.00 0.00 C ATOM 1495 C SER A 103131.329 -16.216 26.219 1.00 0.00 C ATOM 1496 O SER A 103131.152 -17.349 26.666 1.00 0.00 O ATOM 1497 CB SER A 103130.442 -14.924 28.169 1.00 0.00 C ATOM 1498 OG SER A 103130.264 -16.183 28.794 1.00 0.00 O ATOM 1499 H SER A 103128.814 -16.122 25.786 1.00 0.00 H ATOM 1500 HA SER A 103130.808 -14.146 26.209 1.00 0.00 H ATOM 1501 1HB SER A 103131.388 -14.510 28.485 1.00 0.00 H ATOM 1502 2HB SER A 103129.641 -14.267 28.476 1.00 0.00 H ATOM 1503 HG SER A 103129.437 -16.186 29.280 1.00 0.00 H ATOM 1504 N GLY A 104132.292 -15.922 25.352 1.00 0.00 N ATOM 1505 CA GLY A 104133.203 -16.947 24.880 1.00 0.00 C ATOM 1506 C GLY A 104132.655 -17.708 23.689 1.00 0.00 C ATOM 1507 O GLY A 104133.079 -17.416 22.551 1.00 0.00 O ATOM 1508 OXT GLY A 104131.800 -18.596 23.893 1.00 0.00 O ATOM 1509 H GLY A 104132.385 -15.001 25.030 1.00 0.00 H
ATOM 1510 1HA GLY A 104134.137 -16.483 24.598 1.00 0.00 H
ATOM 1511 2HA GLY A 104133.390 -17.645 25.683 1.00 0.00 H
TER 1512 GLY A 104
ENDMDL

Three-Dimensional Structure Coordinate Table 7

ATOM 1 N GLY A 1128.015 1.010 -10.316 1.00 0.00 N ATOM 2 CA GLY A 1127.655 -0.374 -10.731 1.00 0.00 C ATOM 3 C GLY A 1128.389 -1.429 -9.927 1.00 0.00 C ATOM 4 O GLY A 1128.645 -2.528 -10.420 1.00 0.00 O ATOM 5 1H GLY A 1129.039 1.078 -10.148 1.00 0.00 H ATOM 6 2H GLY A 1127.515 1.263 -9.441 1.00 0.00 H ATOM 7 3H GLY A 1127.751 1.686 -11.061 1.00 0.00 H ATOM 8 1HA GLY A 1126.592 -0.512 -10.600 1.00 0.00 H ATOM 9 2HA GLY A 1127.897 -0.499 -11.776 1.00 0.00 H ATOM10 N SER A 2128.728 -1.096 -8.686 1.00 0.00 N ATOM11 CA SER A 2129.437 -2.024 -7.813 1.00 0.00 C ATOM12 C SER A 2128.513 -2.562 -6.726 1.00 0.00 C ATOM13 O SER A 2128.240 -3.761 -6.667 1.00 0.00 O ATOM14 CB SER A 2130.645 -1.334 -7.176 1.00 0.00 C ATOM15 OG SER A 2131.499 -0.785 -8.163 1.00 0.00 O ATOM16 H SER A 2128.496 -0.205 -8.351 1.00 0.00 H ATOM17 HA SER A 2129.783 -2.849 -8.417 1.00 0.00 H ATOM18 1HB SER A 2130.304 -0.538 -6.531 1.00 0.00 H ATOM19 2HB SER A 2131.203 -2.054 -6.594 1.00 0.00 H ATOM20 HG SER A 2132.295 -0.445 -7.746 1.00 0.00 H ATOM21 N SER A 3128.033 -1.668 -5.868 1.00 0.00 N ATOM22 CA SER A 3127.138 -2.053 -4.782 1.00 0.00 C ATOM23 C SER A 3125.816 -1.298 -4.873 1.00 0.00 C ATOM24 O SER A 3125.217 -0.951 -3.856 1.00 0.00 O

ATOM25 CB SER A 3127.799 -1.786 -3.429 1.00 0.00 C ATOM26 OG SER A 3128.587 -0.609 -3.469 1.00 0.00 O ATOM27 H SER A 3128.287 -0.726 -5.966 1.00 0.00 H ATOM28 HA SER A 3126.942 -3.111 -4.873 1.00 0.00 H ATOM29 1HB SER A 3127.036 -1.666 -2.674 1.00 0.00 H ATOM30 2HB SER A 3128.434 -2.620 -3.170 1.00 0.00 H ATOM31 HG SER A 3128.100 0.088 -3.915 1.00 0.00 H ATOM32 N GLY A 4125.367 -1.048 -6.099 1.00 0.00 N ATOM33 CA GLY A 4124.119 -0.335 -6.299 1.00 0.00 C ATOM34 C GLY A 4124.265 1.160 -6.100 1.00 0.00 C ATOM35 O GLY A 4125.326 1.638 -5.697 1.00 0.00 O ATOM36 H GLY A 4125.887 -1.348 -6.873 1.00 0.00 H ATOM37 1HA GLY A 4123.769 -0.521 -7.304 1.00 0.00 H ATOM38 2HA GLY A 4123.386 -0.711 -5.600 1.00 0.00 H ATOM39 N SER A 5123.197 1.900 -6.381 1.00 0.00 N ATOM40 CA SER A 5123.211 3.351 -6.231 1.00 0.00 C ATOM41 C SER A 5122.158 3.804 -5.225 1.00 0.00 C ATOM42 O SER A 5121.565 4.872 -5.369 1.00 0.00 O ATOM43 CB SER A 5122.967 4.027 -7.581 1.00 0.00 C ATOM44 OG SER A 5123.746 5.203 -7.711 1.00 0.00 O ATOM45 H SER A 5122.380 1.460 -6.698 1.00 0.00 H ATOM46 HA SER A 5124.186 3.637 -5.866 1.00 0.00 H ATOM47 1HB SER A 5123.231 3.346 -8.376 1.00 0.00 H ATOM48 2HB SER A 5121.923 4.291 -7.665 1.00 0.00 H ATOM49 HG SER A 5123.666 5.731 -6.914 1.00 0.00 H ATOM50 N SER A 6121.929 2.982 -4.205 1.00 0.00 N ATOM51 CA SER A 6120.947 3.298 -3.175 1.00 0.00 C ATOM52 C SER A 6121.634 3.702 -1.874 1.00 0.00 C ATOM53 O SER A 6122.774 3.317 -1.617 1.00 0.00 O ATOM54 CB SER A 6120.031 2.097 -2.929 1.00 0.00 C ATOM55 OG SER A 6119.317 1.751 -4.103 1.00 0.00 O

ATOM56 H SER A 6122.434 2.144 -4.144 1.00 0.00 H ATOM57 HA SER A 6120.352 4.127 -3.527 1.00 0.00 H ATOM58 1HB SER A 6120.626 1.249 -2.622 1.00 0.00 H ATOM59 2HB SER A 6119.324 2.340 -2.149 1.00 0.00 H ATOM60 HG SER A 6118.645 1.100 -3.888 1.00 0.00 H ATOM61 N GLYA 7120.931 4.481 -1.058 1.00 0.00 N ATOM62 CA GLY A 7121.489 4.925 0.206 1.00 0.00 C ATOM63 C GLY A 7122.446 6.089 0.041 1.00 0.00 C ATOM64 O GLY A 7122.121 7.080 -0.613 1.00 0.00 O ATOM65 H GLY A 7120.027 4.756 -1.316 1.00 0.00 H ATOM66 1HA GLY A 7120.683 5.226 0.857 1.00 0.00 H ATOM67 2HA GLY A 7122.018 4.101 0.663 1.00 0.00 H ATOM68 N LEUA 8123.629 5.969 0.635 1.00 0.00 N ATOM69 CA LEU A 8124.636 7.021 0.551 1.00 0.00 C ATOM70 C LEUA 8125.948 6.474 -0.004 1.00 0.00 C ATOM71 O LEUA 8126.512 5.522 0.535 1.00 0.00 O ATOM72 CB LEU A 8124.873 7.642 1.930 1.00 0.00 C ATOM73 CG LEU A 8123.800 8.630 2.387 1.00 0.00 C ATOM74 CD1 LEU A 8123.646 8.590 3.899 1.00 0.00 C ATOM75 CD2 LEU A 8124.140 10.038 1.920 1.00 0.00 C ATOM76 H LEUA 8123.829 5.155 1.143 1.00 0.00 H ATOM77 HA LEU A 8124.266 7.782 -0.119 1.00 0.00 H ATOM78 1HB LEU A 8124.930 6.843 2.656 1.00 0.00 H ATOM79 2HB LEU A 8125.821 8.158 1.911 1.00 0.00 H ATOM80 HG LEU A 8122.852 8.351 1.948 1.00 0.00 H ATOM81 1HD1 LEU A 8122.870 7.887 4.164 1.00 0.00 H ATOM82 2HD1 LEU A 8123.380 9.572 4.260 1.00 0.00 H ATOM83 3HD1 LEU A 8124.579 8.282 4.347 1.00 0.00 H ATOM84 1HD2 LEU A 8124.270 10.041 0.848 1.00 0.00 H ATOM85 2HD2 LEU A 8125.054 10.363 2.396 1.00 0.00 H ATOM86 3HD2 LEU A 8123.337 10.709 2.187 1.00 0.00 H ATOM87 N ALAA 9126.427 7.081 -1.085 1.00 0.00 N ATOM88 CA ALA A 9127.671 6.655 -1.713 1.00 0.00 C ATOM89 C ALA A 9128.282 7.780 -2.541 1.00 0.00 C ATOM90 O ALAA 9127.588 8.712 -2.947 1.00 0.00 O ATOM91 CB ALA A 9127.430 5.429 -2.580 1.00 0.00 C ATOM92 H ALA A 9125.931 7.834 -1.468 1.00 0.00 H ATOM93 HA ALA A 9128.363 6.381 -0.929 1.00 0.00 H ATOM94 1HB ALA A 9126.713 4.782 -2.099 1.00 0.00 H ATOM95 2HB ALA A 9128.360 4.897 -2.717 1.00 0.00 H ATOM96 3HB ALA A 9127.047 5.738 -3.542 1.00 0.00 H ATOM97 N MET A 10129.585 7.686 -2.786 1.00 0.00 N ATOM98 CA MET A 10130,290 8.696 -3.566 1.00 0.00 C ATOM99 C MET A 10131.574 8.124 -4.163 1.00 0.00 C ATOM 100 O MET A 10132.645 8.223 -3.564 1.00 0.00 O 101 CB META 10130.617 9.909 -2.692 1.00 0.00 C ATOM 102 CG MET A 10129.385 10.644 -2.188 1.00 0.00 C ATOM 103 SD MET A 10129,778 12.268 -1.509 1.00 0.00 S ATOM 104 CE META 10128.986 13.337 -2.709 1.00 0.00 C ATOM 105 H META 10130.084 6.919 -2.434 1.00 0.00 H ATOM 106 HA MET A 10129.641 9.008 -4.370 1.00 0.00 H ATOM 107 1HB MET A 10131.188 9.579 -1.838 1.00 0.00 H ATOM 108 2HB MET A 10131.213 10.602 -3.267 1.00 0.00 H ATOM 109 1HG MET A 10128.697 10.771 -3.010 1.00 0.00 H ATOM 110 2HG MET A 10128.919 10.050 -1.416 1.00 0.00 H ATOM 111 1HE MET A 10128.189 13.886 -2.232 1.00 0.00 H ATOM 112 2HE MET A 10128.582 12.738 -3.512 1.00 0.00 H ATOM 113 3HE MET A 10129.713 14.030 -3.107 1.00 0.00 H **ATOM** 114 N PROA 11131.483 7.516 -5.359 1.00 0.00 N **ATOM** 115 CA PRO A 11132.643 6.928 -6.035 1.00 0.00 C ATOM 116 C PROA 11133.751 7.950 -6.283 1.00 0.00 C ATOM ATOM 117 O PRO A 11134.920 7.684 -6.004 1.00 0.00 O

118 CB PRO A 11132.081 6.413 -7.364 1.00 0.00 C **ATOM ATOM** 119 CG PRO A 11130.608 6.310 -7.156 1.00 0.00 C 120 CD PRO A 11130.246 7.356 -6.140 1.00 0.00 C **ATOM** 121 HA PRO A 11133.046 6.101 -5.469 1.00 0.00 H ATOM **ATOM** 122 1HB PRO A 11132.320 7.112 -8.152 1.00 0.00 H 123 2HB PRO A 11132.514 5.451 -7.589 1.00 0.00 H **ATOM** 124 1HG PRO A 11130.095 6.502 -8.085 1.00 0.00 H ATOM 125 2HG PRO A 11130.359 5.326 -6.786 1.00 0.00 H **ATOM ATOM** 126 1HD PRO A 11129.976 8.280 -6.630 1.00 0.00 H **ATOM** 127 2HD PRO A 11129.437 7.010 -5.514 1.00 0.00 H 128 N PRO A 12133.404 9.140 -6.810 1.00 0.00 N **ATOM ATOM** 129 CA PRO A 12134.388 10.193 -7.083 1.00 0.00 C 130 C PROA 12135.197 10.557 -5.844 1.00 0.00 C ATOM **ATOM** 131 O PROA 12136.300 11.094 -5.944 1.00 0.00 O **ATOM** 132 CB PRO A 12133.533 11.382 -7.530 1.00 0.00 C 133 CG PRO A 12132.261 10.781 -8.015 1.00 0.00 C ATOM 134 CD PRO A 12132.036 9.557 -7.172 1.00 0.00 C **ATOM** 135 HA PRO A 12135.060 9.908 -7.880 1.00 0.00 H **ATOM** 136 1HB PRO A 12133.364 12.042 -6.691 1.00 0.00 H **ATOM ATOM** 137 2HB PRO A 12134.040 11.918 -8.318 1.00 0.00 H 138 1HG PRO A 12131.450 11.481 -7.884 1.00 0.00 H **ATOM** 139 2HG PRO A 12132.357 10.506 -9.055 1.00 0.00 H ATOM 140 1HD PRO A 12131.462 9.806 -6.292 1.00 0.00 H **ATOM ATOM** 141 2HD PRO A 12131.537 8.792 -7.746 1.00 0.00 H 142 N GLY A 13134.641 10.259 -4.673 1.00 0.00 N ATOM **ATOM** 143 CA GLY A 13135.325 10.562 -3.429 1.00 0.00 C 144 C GLYA 13136.013 9.350 -2.835 1.00 0.00 C **ATOM** 145 O GLY A 13135.664 8.902 -1.743 1.00 0.00 O **ATOM** 146 H GLY A 13133.758 9.830 -4.653 1.00 0.00 H **ATOM** 147 1HA GLY A 13136.063 11.328 -3.615 1.00 0.00 H **ATOM** 148 2HA GLY A 13134.604 10.938 -2.717 1.00 0.00 H ATOM

- ATOM 149 N ASN A 14136.995 8.818 -3.554 1.00 0.00 N
- ATOM 150 CA ASN A 14137.736 7.650 -3.092 1.00 0.00 C
- ATOM 151 C ASN A 14136.803 6.459 -2.890 1.00 0.00 C
- ATOM 152 O ASN A 14136.816 5.818 -1.839 1.00 0.00 O
- ATOM 153 CB ASN A 14138.469 7.970 -1.786 1.00 0.00 C
- ATOM 154 CG ASN A 14139.436 9.126 -1.935 1.00 0.00 C
- ATOM 155 OD1 ASN A 14140.104 9.265 -2.961 1.00 0.00 O
- ATOM 156 ND2 ASN A 14139.519 9.965 -0.909 1.00 0.00 N
- ATOM 157 H ASN A 14137.228 9.220 -4.417 1.00 0.00 H
- ATOM 158 HA ASN A 14138.463 7.398 -3.848 1.00 0.00 H
- ATOM 159 1HB ASN A 14137.743 8.227 -1.028 1.00 0.00 H
- ATOM 160 2HB ASN A 14139.022 7.098 -1.468 1.00 0.00 H
- ATOM 161 1HD2 ASN A 14138.958 9.793 -0.124 1.00 0.00 H
- ATOM 162 2HD2 ASN A 14140.137 10.722 -0.978 1.00 0.00 H
- ATOM 163 N SER A 15135.996 6.168 -3.905 1.00 0.00 N
- ATOM 164 CA SER A 15135.055 5.054 -3.844 1.00 0.00 C
- ATOM 165 C SER A 15134.001 5.290 -2.766 1.00 0.00 C
- ATOM 166 O SER A 15132.873 5.682 -3.063 1.00 0.00 O
- ATOM 167 CB SER A 15135.798 3.742 -3.575 1.00 0.00 C
- ATOM 168 OG SER A 15136.062 3.049 -4.783 1.00 0.00 O
- ATOM 169 H SER A 15136.034 6.716 -4.718 1.00 0.00 H
- ATOM 170 HA SER A 15134.562 4.986 -4.802 1.00 0.00 H
- ATOM 171 1HB SER A 15136.736 3.957 -3.085 1.00 0.00 H
- ATOM 172 2HB SER A 15135.194 3.114 -2.938 1.00 0.00 H
- ATOM 173 HG SER A 15136.234 2.124 -4.589 1.00 0.00 H
- ATOM 174 N HIS A 16134.376 5.049 -1.514 1.00 0.00 N
- ATOM 175 CA HIS A 16133.462 5.237 -0.393 1.00 0.00 C
- ATOM 176 C HIS A 16134.143 5.997 0.742 1.00 0.00 C
- ATOM 177 O HIS A 16133.685 7.064 1.150 1.00 0.00 O
- ATOM 178 CB HIS A 16132.957 3.883 0.113 1.00 0.00 C
- ATOM 179 CG HIS A 16131.570 3.555 -0.342 1.00 0.00 C

180 ND1 HIS A 16130.456 3.728 0.453 1.00 0.00 N **ATOM** 181 CD2 HIS A 16131.115 3.061 -1.519 1.00 0.00 C **ATOM ATOM** 182 CE1 HIS A 16129.377 3.355 -0.214 1.00 0.00 C 183 NE2 HIS A 16129.751 2.947 -1.413 1.00 0.00 N ATOM 184 H HIS A 16135.289 4.740 -1.339 1.00 0.00 H **ATOM ATOM** 185 HA HIS A 16132.622 5.817 -0.744 1.00 0.00 H 186 1HB HIS A 16133.616 3.105 -0.245 1.00 0.00 H **ATOM** 187 2HB HIS A 16132.962 3.883 1.193 1.00 0.00 H **ATOM** 188 HD1 HIS A 16130.456 4.074 1.370 1.00 0.00 H ATOM **ATOM** 189 HD2 HIS A 16131.715 2.805 -2.381 1.00 0.00 H 190 HE1 HIS A 16128.364 3.381 0.158 1.00 0.00 H ATOM ATOM 191 HE2 HIS A 16129.161 2.533 -2.078 1.00 0.00 H 192 N GLY A 17135.238 5.440 1.246 1.00 0.00 N **ATOM ATOM** 193 CA GLY A 17135.964 6.079 2.329 1.00 0.00 C 194 C GLY A 17137.320 5.446 2.570 1.00 0.00 C **ATOM** 195 O GLY A 17137.588 4.929 3.654 1.00 0.00 O **ATOM ATOM** 196 H GLY A 17135.557 4.588 0.881 1.00 0.00 H **ATOM** 197 1HA GLY A 17136.104 7.122 2.087 1.00 0.00 H 198 2HA GLY A 17135.378 6.004 3.233 1.00 0.00 H **ATOM** 199 N LEUA 18138.179 5.487 1.556 1.00 0.00 N **ATOM** 200 CA LEU A 18139.516 4.914 1.663 1.00 0.00 C ATOM 201 C LEUA 18140.514 5.950 2.171 1.00 0.00 C **ATOM** 202 O LEUA 18140.889 6.873 1.448 1.00 0.00 O ATOM 203 CB LEU A 18139.972 4.374 0.306 1.00 0.00 C ATOM 204 CG LEUA 18138.938 3.521 -0.431 1.00 0.00 C ATOM 205 CD1 LEU A 18139.197 3.545 -1.929 1.00 0.00 C ATOM 206 CD2 LEU A 18138.957 2.092 0.092 1.00 0.00 C ATOM 207 H LEUA 18137.907 5.914 0.717 1.00 0.00 H ATOM 208 HA LEUA 18139.471 4.098 2.369 1.00 0.00 H **ATOM** 209 1HB LEU A 18140.231 5.213 -0.323 1.00 0.00 H ATOM ATOM 210 2HB LEU A 18140.856 3.774 0.460 1.00 0.00 H

211 HG LEUA 18137.954 3.929 -0.256 1.00 0.00 H 212 1HD1 LEU A 18138.664 2.732 -2.399 1.00 0.00 H **ATOM** 213 2HD1 LEU A 18140.255 3.436 -2.114 1.00 0.00 H **ATOM** 214 3HD1 LEU A 18138.855 4.484 -2.338 1.00 0.00 H **ATOM** 215 1HD2 LEU A 18139.980 1.770 0.220 1.00 0.00 H ATOM 216 2HD2 LEU A 18138.461 1.443 -0.615 1.00 0.00 H ATOM ATOM 217 3HD2 LEU A 18138.445 2.050 1.041 1.00 0.00 H **ATOM** 218 N GLUA 19140.937 5.792 3.420 1.00 0.00 N 219 CA GLUA 19141.892 6.714 4.026 1.00 0.00 C **ATOM** 220 C GLUA 19142.828 5.978 4.980 1.00 0.00 C ATOM 221 O GLUA 19142.700 4.771 5.184 1.00 0.00 O ATOM ATOM 222 CB GLUA 19141.153 7.825 4.774 1.00 0.00 C 223 CG GLU A 19140.096 7.312 5.737 1.00 0.00 C ATOM 224 CD GLUA 19140.078 8.078 7.045 1.00 0.00 C ATOM 225 OE1 GLU A 19139.086 8.792 7.302 1.00 0.00 O ATOM 226 OE2 GLU A 19141.056 7.963 7.814 1.00 0.00 O ATOM 227 H GLUA 19140.601 5.037 3.947 1.00 0.00 H ATOM 228 HA GLU A 19142.478 7.153 3.233 1.00 0.00 H ATOM 229 1HB GLU A 19141.872 8.403 5.336 1.00 0.00 H ATOM 230 2HB GLU A 19140.672 8.469 4.053 1.00 0.00 H **ATOM** 231 1HG GLU A 19139.127 7.406 5.270 1.00 0.00 H ATOM 232 2HG GLU A 19140.294 6.271 5.948 1.00 0.00 H **ATOM** 233 N VALA 20143.770 6.715 5.562 1.00 0.00 N ATOM 234 CA VALA 20144.726 6.133 6.495 1.00 0.00 C **ATOM** 235 C VALA 20144.014 5.482 7.678 1.00 0.00 C ATOM 236 O VAL A 20143.052 6.032 8.215 1.00 0.00 O **ATOM** 237 CB VALA 20145.712 7.194 7.023 1.00 0.00 C **ATOM** 238 CG1 VAL A 20146.786 6.547 7.885 1.00 0.00 C **ATOM** 239 CG2 VAL A 20146.337 7.962 5.868 1.00 0.00 C **ATOM** 240 H VALA 20143.820 7.673 5.360 1.00 0.00 H **ATOM** 241 HA VALA 20145.291 5.378 5.968 1.00 0.00 H ATOM

242 HB VALA 20145.162 7.893 7.636 1.00 0.00 H ATOM 243 1HG1 VAL A 20146.375 6.316 8.857 1.00 0.00 H 244 2HG1 VAL A 20147.615 7.229 7.999 1.00 0.00 H ATOM 245 3HG1 VAL A 20147.129 5.638 7.413 1.00 0.00 H ATOM 246 1HG2 VAL A 20147.314 8.318 6.159 1.00 0.00 H **ATOM** 247 2HG2 VAL A 20145.708 8.802 5.613 1.00 0.00 H **ATOM** 248 3HG2 VAL A 20146.431 7.310 5.012 1.00 0.00 H ATOM 249 N GLY A 21144.493 4.309 8.077 1.00 0.00 N **ATOM** 250 CA GLY A 21143.890 3.603 9.192 1.00 0.00 C **ATOM** 251 C GLY A 21142.852 2.592 8.746 1.00 0.00 C **ATOM** 252 O GLY A 21142.800 1.477 9.261 1.00 0.00 O **ATOM** 253 H GLY A 21145.263 3.919 7.611 1.00 0.00 H **ATOM** 254 1HA GLY A 21144.666 3.088 9.740 1.00 0.00 H **ATOM** 255 2HA GLY A 21143.419 4.321 9.846 1.00 0.00 H ATOM 256 N SER A 22142.024 2.985 7.783 1.00 0.00 N **ATOM** 257 CA SER A 22140.981 2.106 7.266 1.00 0.00 C **ATOM** 258 C SER A 22141.573 1.041 6.348 1.00 0.00 C **ATOM** 259 O SER A 22142.497 1.314 5.581 1.00 0.00 O **ATOM** 260 CB SER A 22139.928 2.918 6.510 1.00 0.00 C **ATOM** 261 OG SER A 22139.576 4.090 7.227 1.00 0.00 O **ATOM** 262 H SER A 22142.115 3.887 7.412 1.00 0.00 H ATOM 263 HA SER A 22140.512 1.619 8.107 1.00 0.00 H **ATOM** 264 1HB SER A 22140.321 3.206 5.547 1.00 0.00 H ATOM -**ATOM** 265 2HB SER A 22139.042 2.316 6.372 1.00 0.00 H 266 HG SER A 22140.307 4.712 7.202 1.00 0.00 H ATOM 267 N LEUA 23141.037 -0.171 6.433 1.00 0.00 N **ATOM** 268 CA LEU A 23141.513 -1.277 5.610 1.00 0.00 C ATOM 269 C LEUA 23141.115 -1.081 4.150 1.00 0.00 C ATOM 270 O LEUA 23140.071 -0.500 3.854 1.00 0.00 O ATOM 271 CB LEU A 23140.956 -2.603 6.129 1.00 0.00 C **ATOM** ATOM 272 CG LEU A 23141.330 -2.942 7.574 1.00 0.00 C

ATOM 273 CD1 LEU A 23140.251 -3.798 8.217 1.00 0.00 C 274 CD2 LEU A 23142.675 -3.649 7.623 1.00 0.00 C 275 H LEU A 23140.303 -0.327 7.064 1.00 0.00 H 276 HA LEUA 23142.590 -1.299 5.677 1.00 0.00 H **ATOM** 277 1HB LEU A 23139.878 -2.570 6.056 1.00 0.00 H **ATOM** 278 2HB LEU A 23141.319 -3.396 5.492 1.00 0.00 H 279 HG LEUA 23141.411 -2.026 8.140 1.00 0.00 H **ATOM** 280 1HD1 LEU A 23140.197 -3.576 9.273 1.00 0.00 H **ATOM** 281 2HD1 LEU A 23140.490 -4.843 8.080 1.00 0.00 H **ATOM** 282 3HD1 LEU A 23139.298 -3.584 7.756 1.00 0.00 H **ATOM** 283 1HD2 LEU A 23143.218 -3.332 8.501 1.00 0.00 H ATOM 284 2HD2 LEU A 23143.245 -3.402 6.739 1.00 0.00 H **ATOM** 285 3HD2 LEU A 23142.519 -4.718 7.662 1.00 0.00 H **ATOM** 286 N ALAA 24141.955 -1.570 3.243 1.00 0.00 N ATOM 287 CA ALAA 24141.691 -1.451 1.815 1.00 0.00 C ATOM 288 C ALAA 24142.305 -2.615 1.045 1.00 0.00 C **ATOM** 289 O ALAA 24143.292 -3.209 1.480 1.00 0.00 O **ATOM** 290 CB ALAA 24142.226 -0.127 1.289 1.00 0.00 C **ATOM** 291 H ALAA 24142.771 -2.023 3.542 1.00 0.00 H ATOM 292 HA ALA A 24140.621 -1.462 1.671 1.00 0.00 H ATOM 293 1HB ALA A 24142.507 -0.239 0.251 1.00 0.00 H **ATOM** 294 2HB ALA A 24143.091 0.166 1.866 1.00 0.00 H ATOM 295 3HB ALA A 24141.461 0.630 1.375 1.00 0.00 H **ATOM** 296 N GLUA 25141.715 -2.937 -0.102 1.00 0.00 N **ATOM** 297 CA GLU A 25142.205 -4.032 -0.932 1.00 0.00 C ATOM 298 C GLUA 25142.605 -3.530 -2.316 1.00 0.00 C **ATOM** 299 O GLU A 25142.089 -2.519 -2.793 1.00 0.00 O ATOM 300 CB GLUA 25141.136 -5.119 -1.062 1.00 0.00 C **ATOM** 301 CG GLUA 25141.708 -6.516 -1.245 1.00 0.00 C ATOM **ATOM** 302 CD GLUA 25140.729 -7.464 -1.909 1.00 0.00 C 303 OE1 GLU A 25139.929 -6.999 -2.749 1.00 0.00 O

- ATOM 304 OE2 GLU A 25140.762 -8.671 -1.590 1.00 0.00 O
- ATOM 305 H GLUA 25140.932 -2.428 -0.396 1.00 0.00 H
- ATOM 306 HA GLU A 25143.075 -4.452 -0.449 1.00 0.00 H
- ATOM 307 1HB GLU A 25140.527 -5.117 -0.170 1.00 0.00 H
- ATOM 308 2HB GLU A 25140.512 -4.894 -1.915 1.00 0.00 H
- ATOM 309 1HG GLU A 25142.594 -6.451 -1.858 1.00 0.00 H
- ATOM 310 2HG GLU A 25141.970 -6.913 -0.275 1.00 0.00 H
- ATOM 311 N VALA 26143.528 -4.243 -2.954 1.00 0.00 N
- ATOM 312 CA VAL A 26143.998 -3.869 -4.282 1.00 0.00 C
- ATOM 313 C VALA 26143.826 -5.020 -5.268 1.00 0.00 C
- ATOM 314 O VALA 26144.136 -6.170 -4.955 1.00 0.00 O
- ATOM 315 CB VALA 26145.480 -3.446 -4.258 1.00 0.00 C
- ATOM 316 CG1 VAL A 26145.909 -2.913 -5.616 1.00 0.00 C
- ATOM 317 CG2 VAL A 26145.722 -2.410 -3.170 1.00 0.00 C
- ATOM 318 H VALA 26143.901 -5.039 -2.521 1.00 0.00 H
- ATOM 319 HA VALA 26143.411 -3.027 -4.621 1.00 0.00 H
- ATOM 320 HB VAL A 26146.078 -4.318 -4.033 1.00 0.00 H
- ATOM 321 1HG1 VAL A 26145.900 -1.833 -5.598 1.00 0.00 H
- ATOM 322 2HG1 VAL A 26145.225 -3.266 -6.374 1.00 0.00 H
- ATOM 323 3HG1 VAL A 26146.905 -3.261 -5.841 1.00 0.00 H
- ATOM 324 1HG2 VAL A 26146.651 -2.631 -2.663 1.00 0.00 H
- ATOM 325 2HG2 VAL A 26144.909 -2.434 -2.460 1.00 0.00 H
- ATOM 326 3HG2 VAL A 26145.781 -1.428 -3.616 1.00 0.00 H
- ATOM 327 N LYS A 27143.330 -4.704 -6.460 1.00 0.00 N
- ATOM 328 CA LYS A 27143.116 -5.712 -7.491 1.00 0.00 C
- ATOM 329 C LYS A 27144.437 -6.118 -8.137 1.00 0.00 C
- ATOM 330 O LYS A 27144.790 -5.631 -9.211 1.00 0.00 O
- ATOM 331 CB LYS A 27142.155 -5.184 -8.558 1.00 0.00 C
- ATOM 332 CG LYS A 27140.694 -5.475 -8.257 1.00 0.00 C
- ATOM 333 CD LYS A 27139.793 -4.342 -8.722 1.00 0.00 C
- ATOM 334 CE LYS A 27138.436 -4.857 -9.172 1.00 0.00 C

ATOM 335 NZ LYS A 27137.427 -4.798 -8.079 1.00 0.00 N 336 H LYS A 27143.102 -3.769 -6.649 1.00 0.00 H **ATOM** 337 HA LYS A 27142.677 -6.579 -7.021 1.00 0.00 H **ATOM** 338 1HB LYS A 27142.277 -4.114 -8.639 1.00 0.00 H **ATOM** 339 2HB LYS A 27142.403 -5.638 -9.506 1.00 0.00 H ATOM **ATOM** 340 1HG LYS A 27140.405 -6.382 -8.767 1.00 0.00 H 341 2HG LYS A 27140.574 -5.604 -7.192 1.00 0.00 H ATOM **ATOM** 342 1HD LYS A 27139.650 -3.651 -7.905 1.00 0.00 H **ATOM** 343 2HD LYS A 27140.268 -3.833 -9.549 1.00 0.00 H **ATOM** 344 1HE LYS A 27138.092 -4.255 -10.000 1.00 0.00 H 345 2HE LYS A 27138.544 -5.883 -9.497 1.00 0.00 H **ATOM** 346 1HZ LYS A 27136.494 -4.552 -8.466 1.00 0.00 H **ATOM** 347 2HZ LYS A 27137.700 -4.079 -7.379 1.00 0.00 H **ATOM** 348 3HZ LYS A 27137.361 -5.721 -7.603 1.00 0.00 H **ATOM** 349 N GLUA 28145.162 -7.014 -7.475 1.00 0.00 N **ATOM ATOM** 350 CA GLU A 28146.444 -7.487 -7.986 1.00 0.00 C **ATOM** 351 C GLUA 28146.465 -9.010 -8.076 1.00 0.00 C 352 O GLUA 28145.504 -9.678 -7.694 1.00 0.00 O ATOM 353 CB GLUA 28147.585 -6.998 -7.090 1.00 0.00 C **ATOM ATOM** 354 CG GLUA 28148.729 -6.358 -7.858 1.00 0.00 C 355 CD GLUA 28149.850 -5.889 -6.951 1.00 0.00 C **ATOM** 356 OE1 GLU A 28150.027 -4.661 -6.811 1.00 0.00 O **ATOM** 357 OE2 GLU A 28150.550 -6.751 -6.378 1.00 0.00 O **ATOM** 358 H GLUA 28144.828 -7.367 -6.625 1.00 0.00 H **ATOM** 359 HA GLUA 28146.577 -7.079 -8.976 1.00 0.00 H **ATOM** 360 1HB GLU A 28147.195 -6.271 -6.394 1.00 0.00 H ATOM **ATOM** 361 2HB GLU A 28147.979 -7.838 -6.535 1.00 0.00 H 362 1HG GLU A 28149.129 -7.080 -8.553 1.00 0.00 H ATOM 363 2HG GLU A 28148.348 -5.507 -8.404 1.00 0.00 H ATOM ATOM 364 N ASNA 29147.568 -9.551 -8.582 1.00 0.00 N 365 CA ASN A 29147.716 -10.996 -8.721 1.00 0.00 C ATOM

- ATOM 366 C ASN A 29147.613 -11.688 -7.363 1.00 0.00 C
- ATOM 367 O ASN A 29146.752 -12.543 -7.158 1.00 0.00 O
- ATOM 368 CB ASN A 29149.055 -11.331 -9.380 1.00 0.00 C
- ATOM 369 CG ASN A 29148.926 -11.543 -10.876 1.00 0.00 C
- ATOM 370 OD1 ASN A 29149.065 -12.662 -11.371 1.00 0.00 O
- ATOM 371 ND2 ASN A 29148.660 -10.465 -11.605 1.00 0.00 N
- ATOM 372 H ASN A 29148.301 -8.967 -8.868 1.00 0.00 H
- ATOM 373 HA ASN A 29146.915 -11.351 -9.353 1.00 0.00 H
- ATOM 374 1HB ASN A 29149.747 -10.520 -9.210 1.00 0.00 H
- ATOM 375 2HB ASN A 29149.451 -12.235 -8.939 1.00 0.00 H
- ATOM 376 1HD2 ASN A 29148.563 -9.606 -11.144 1.00 0.00 H
- ATOM 377 2HD2 ASN A 29148.571 -10.574 -12.575 1.00 0.00 H
- ATOM 378 N PRO A 30148.497 -11.327 -6.416 1.00 0.00 N
- ATOM 379 CA PRO A 30148.502 -11.917 -5.076 1.00 0.00 C
- ATOM 380 C PRO A 30147.380 -11.368 -4.195 1.00 0.00 C
- ATOM 381 O PRO A 30147.416 -10.208 -3.786 1.00 0.00 O
- ATOM 382 CB PRO A 30149.865 -11.505 -4.521 1.00 0.00 C
- ATOM 383 CG PRO A 30150.175 -10.219 -5.206 1.00 0.00 C
- ATOM 384 CD PRO A 30149.559 -10.314 -6.578 1.00 0.00 C
- ATOM 385 HA PRO A 30148.437 -12.993 -5.117 1.00 0.00 H
- ATOM 386 1HB PRO A 30149.797 -11.378 -3.450 1.00 0.00 H
- ATOM 387 2HB PRO A 30150.597 -12.263 -4.755 1.00 0.00 H
- ATOM 388 1HG PRO A 30149.739 -9.397 -4.657 1.00 0.00 H
- ATOM 389 2HG PRO A 30151.244 -10.094 -5.285 1.00 0.00 H
- ATOM 390 1HD PRO A 30149.142 -9.362 -6.870 1.00 0.00 H
- ATOM 391 2HD PRO A 30150.294 -10.640 -7.298 1.00 0.00 H
- ATOM 392 N PRO A 31146.363 -12.196 -3.889 1.00 0.00 N
- ATOM 393 CA PRO A 31145.234 -11.777 -3.052 1.00 0.00 C
- ATOM 394 C PRO A 31145.642 -11.550 -1.601 1.00 0.00 C
- ATOM 395 O PRO A 31145.519 -12.444 -0.764 1.00 0.00 O
- ATOM 396 CB PRO A 31144.257 -12.951 -3.155 1.00 0.00 C

397 CG PRO A 31145.111 -14.127 -3.484 1.00 0.00 C 398 CD PRO A 31146.234 -13.598 -4.331 1.00 0.00 C **ATOM** 399 HA PRO A 31144.767 -10.882 -3.438 1.00 0.00 H ATOM 400 1HB PRO A 31143.748 -13.083 -2.212 1.00 0.00 H **ATOM** 401 2HB PRO A 31143.537 -12.757 -3.936 1.00 0.00 H ATOM 402 1HG PRO A 31145.499 -14.563 -2.575 1.00 0.00 H **ATOM ATOM** 403 2HG PRO A 31144.536 -14.855 -4.037 1.00 0.00 H 404 1HD PRO A 31147.143 -14.148 -4.138 1.00 0.00 H **ATOM** 405 2HD PRO A 31145.974 -13.649 -5.378 1.00 0.00 H **ATOM** 406 N PHE A 32146.130 -10.348 -1.310 1.00 0.00 N **ATOM** 407 CA PHE A 32146.557 -10.002 0.040 1.00 0.00 C **ATOM** 408 C PHE A 32145.562 -9.052 0.699 1.00 0.00 C **ATOM** 409 O PHE A 32144.630 -8.569 0.056 1.00 0.00 O ATOM 410 CB PHE A 32147.947 -9.364 0.009 1.00 0.00 C **ATOM** 411 CG PHE A 32148.016 -8.116 -0.824 1.00 0.00 C **ATOM** 412 CD1 PHE A 32148.649 -8.124 -2.056 1.00 0.00 C ATOM 413 CD2 PHE A 32147.447 -6.935 -0.374 1.00 0.00 C **ATOM** 414 CE1 PHE A 32148.713 -6.978 -2.825 1.00 0.00 C ATOM 415 CE2 PHE A 32147.508 -5.785 -1.139 1.00 0.00 C ATOM 416 CZ PHE A 32148.143 -5.807 -2.366 1.00 0.00 C **ATOM** 417 H PHE A 32146.203 -9.678 -2.022 1.00 0.00 H **ATOM** 418 HA PHE A 32146.602 -10.913 0.617 1.00 0.00 H **ATOM** 419 1HB PHE A 32148.240 -9.107 1.017 1.00 0.00 H **ATOM** 420 2HB PHE A 32148.652 -10.075 -0.395 1.00 0.00 H ATOM 421 HD1 PHE A 32149.095 -9.039 -2.416 1.00 0.00 H **ATOM** 422 HD2 PHE A 32146.950 -6.918 0.584 1.00 0.00 H ATOM 423 HE1 PHE A 32149.211 -6.997 -3.784 1.00 0.00 H ATOM 424 HE2 PHE A 32147.060 -4.872 -0.778 1.00 0.00 H ATOM 425 HZ PHE A 32148.192 -4.910 -2.965 1.00 0.00 H **ATOM** 426 N TYR A 33145.770 -8.785 1.984 1.00 0.00 N ATOM ATOM 427 CA TYR A 33144.892 -7.892 2.731 1.00 0.00 C

ATOM 428 C TYR A 33145.696 -7.001 3.673 1.00 0.00 C 429 O TYR A 33146.335 -7.487 4.607 1.00 0.00 O 430 CB TYR A 33143.865 -8.699 3.527 1.00 0.00 C ATOM ATOM 431 CG TYR A 33142.662 -9.121 2.712 1.00 0.00 C ATOM 432 CD1 TYR A 33141.948 -8.193 1.962 1.00 0.00 C ATOM 433 CD2 TYR A 33142.243 -10.444 2.691 1.00 0.00 C ATOM 434 CE1 TYR A 33140.848 -8.576 1.217 1.00 0.00 C 435 CE2 TYR A 33141.145 -10.833 1.947 1.00 0.00 C ATOM 436 CZ TYR A 33140.452 -9.896 1.212 1.00 0.00 C ATOM 437 OH TYR A 33139.358 -10.279 0.469 1.00 0.00 O ATOM 438 H TYR A 33146.531 -9.200 2.442 1.00 0.00 H ATOM 439 HA TYR A 33144.373 -7.267 2.020 1.00 0.00 H ATOM **ATOM** 440 1HB TYR A 33144.335 -9.592 3.908 1.00 0.00 H 441 2HB TYR A 33143.512 -8.102 4.355 1.00 0.00 H ATOM ATOM 442 HD1 TYR A 33142.261 -7.160 1.968 1.00 0.00 H 443 HD2 TYR A 33142.788 -11.177 3.268 1.00 0.00 H ATOM 444 HE1 TYR A 33140.306 -7.840 0.641 1.00 0.00 H **ATOM** 445 HE2 TYR A 33140.835 -11.869 1.943 1.00 0.00 H ATOM 446 HH TYR A 33139.593 -11.028 -0.083 1.00 0.00 H ATOM 447 N GLY A 34145.660 -5.697 3.422 1.00 0.00 N ATOM 448 CA GLY A 34146.389 -4.761 4.257 1.00 0.00 C ATOM 449 C GLY A 34145.568 -3.537 4.613 1.00 0.00 C **ATOM** 450 O GLY A 34144.380 -3.465 4.294 1.00 0.00 O **ATOM** 451 H GLY A 34145.133 -5.368 2.664 1.00 0.00 H **ATOM** 452 1HA GLY A 34146.683 -5.260 5.168 1.00 0.00 H ATOM 453 2HA GLY A 34147.278 -4.443 3.731 1.00 0.00 H **ATOM** ATOM 454 N VALA 35146.200 -2.573 5.275 1.00 0.00 N 455 CA VALA 35145.520 -1.348 5.674 1.00 0.00 C ATOM 456 C VALA 35146.266 -0.117 5.168 1.00 0.00 C ATOM 457 O VALA 35147.494 -0.110 5.093 1.00 0.00 O ATOM

ATOM 458 CB VALA 35145.376 -1.261 7.207 1.00 0.00 C

459 CG1 VAL A 35146.742 -1.264 7.877 1.00 0.00 C ATOM 460 CG2 VALA 35144.581 -0.024 7.601 1.00 0.00 C ATOM 461 H VALA 35147.147 -2.690 5.499 1.00 0.00 H ATOM **ATOM** 462 HA VALA 35144.531 -1.360 5.241 1.00 0.00 H 463 HB VALA 35144.834 -2.131 7.546 1.00 0.00 H **ATOM** 464 1HG1 VAL A 35146.735 -0.577 8.711 1.00 0.00 H **ATOM** 465 2HG1 VAL A 35147.493 -0.959 7.165 1.00 0.00 H **ATOM** 466 3HG1 VAL A 35146.965 -2.258 8.232 1.00 0.00 H **ATOM** 467 1HG2 VAL A 35144.998 0.843 7.113 1.00 0.00 H **ATOM** 468 2HG2 VAL A 35144.629 0.108 8.672 1.00 0.00 H **ATOM** 469 3HG2 VAL A 35143.551 -0.146 7.300 1.00 0.00 H **ATOM** 470 N ILEA 36145.515 0.923 4.822 1.00 0.00 N **ATOM ATOM** 471 CA ILE A 36146.105 2.160 4.324 1.00 0.00 C 472 C ILE A 36147.035 2.779 5.362 1.00 0.00 C **ATOM** 473 O ILE A 36146.862 2.574 6.564 1.00 0.00 O **ATOM** 474 CB ILE A 36145.023 3.188 3.939 1.00 0.00 C ATOM 475 CG1 ILE A 36144.010 2.562 2.977 1.00 0.00 C **ATOM** 476 CG2 ILE A 36145.660 4.422 3.315 1.00 0.00 C ATOM 477 CD1 ILE A 36142.915 3.515 2.548 1.00 0.00 C **ATOM** 478 H ILE A 36144.540 0.859 4.905 1.00 0.00 H **ATOM** 479 HA ILE A 36146.678 1.923 3.439 1.00 0.00 H **ATOM** 480 HB ILE A 36144.512 3.494 4.840 1.00 0.00 H **ATOM** 481 1HG1 ILE A 36144.525 2.229 2.089 1.00 0.00 H **ATOM ATOM** 482 2HG1 ILE A 36143.544 1.715 3.457 1.00 0.00 H 483 1HG2 ILE A 36146.128 5.015 4.087 1.00 0.00 H ATOM 484 2HG2 ILE A 36144.900 5.009 2.822 1.00 0.00 H **ATOM** 485 3HG2 ILE A 36146.404 4.117 2.593 1.00 0.00 H ATOM 486 1HD1 ILE A 36142.149 3.548 3.308 1.00 0.00 H **ATOM** 487 2HD1 ILE A 36142.486 3.173 1.617 1.00 0.00 H ATOM 488 3HD1 ILE A 36143.330 4.502 2.412 1.00 0.00 H **ATOM** 489 N ARGA 37148.020 3.537 4.891 1.00 0.00 N ATOM

490 CA ARG A 37148.977 4.184 5.780 1.00 0.00 C ATOM 491 C ARG A 37149.216 5.631 5.364 1.00 0.00 C ATOM 492 O ARG A 37148.844 6.563 6.078 1.00 0.00 O ATOM 493 CB ARG A 37150.300 3.418 5.782 1.00 0.00 C ATOM 494 CG ARG A 37150.144 1.935 6.077 1.00 0.00 C **ATOM** 495 CD ARG A 37150.115 1.667 7.572 1.00 0.00 C **ATOM** 496 NE ARG A 37148.908 2.196 8.201 1.00 0.00 N ATOM **ATOM** 497 CZ ARG A 37148.788 2.420 9.508 1.00 0.00 C **ATOM** 498 NH1 ARG A 37149.800 2.159 10.327 1.00 0.00 N 499 NH2 ARG A 37147.654 2.904 9.997 1.00 0.00 N ATOM 500 H ARG A 37148.105 3.662 3.924 1.00 0.00 H ATOM 501 HA ARG A 37148.563 4.173 6.778 1.00 0.00 H ATOM 502 1HB ARG A 37150.766 3.523 4.813 1.00 0.00 H **ATOM** 503 2HB ARG A 37150,950 3.845 6.532 1.00 0.00 H **ATOM** 504 1HG ARG A 37149.220 1.587 5.641 1.00 0.00 H **ATOM** 505 2HG ARG A 37150.976 1.402 5.640 1.00 0.00 H ATOM 506 1HD ARG A 37150.154 0.600 7.734 1.00 0.00 H **ATOM** 507 2HD ARG A 37150.979 2.130 8.025 1.00 0.00 H **ATOM** 508 HE ARG A 37148.145 2.397 7.619 1.00 0.00 H ATOM 509 1HH1 ARG A 37150.657 1.793 9.966 1.00 0.00 H **ATOM** 510 2HH1 ARG A 37149.704 2.329 11.308 1.00 0.00 H ATOM 511 1HH2 ARG A 37146.890 3.103 9.384 1.00 0.00 H ATOM 512 2HH2 ARG A 37147.565 3.072 10.979 1.00 0.00 H ATOM 513 N TRP A 38149.841 5.814 4.206 1.00 0.00 N ATOM 514 CA TRPA 38150.132 7.149 3.697 1.00 0.00 C **ATOM** 515 C TRP A 38149.473 7.373 2.337 1.00 0.00 C **ATOM** 516 O TRP A 38149.599 6.550 1.431 1.00 0.00 O ATOM 517 CB TRP A 38151.647 7.361 3.589 1.00 0.00 C ATOM 518 CG TRP A 38152.027 8.592 2.820 1.00 0.00 C ATOM 519 CD1 TRP A 38152.264 9.837 3.329 1.00 0.00 C **ATOM** 520 CD2 TRP A 38152.208 8.696 1.403 1.00 0.00 C ATOM

521 NE1 TRP A 38152.581 10.708 2.314 1.00 0.00 N ATOM 522 CE2 TRP A 38152.554 10.031 1.123 1.00 0.00 C ATOM 523 CE3 TRP A 38152.112 7.789 0.344 1.00 0.00 C ATOM 524 CZ2 TRP A 38152.803 10.479 -0.172 1.00 0.00 C ATOM 525 CZ3 TRP A 38152.360 8.234 -0.940 1.00 0.00 C 526 CH2 TRP A 38152.702 9.569 -1.189 1.00 0.00 C **ATOM** 527 H TRPA 38150.114 5.032 3.682 1.00 0.00 H ATOM 528 HA TRP A 38149.728 7.865 4.398 1.00 0.00 H ATOM **ATOM** 529 1HB TRP A 38152.062 7.447 4.581 1.00 0.00 H 530 2HB TRP A 38152.086 6.508 3.092 1.00 0.00 H ATOM 531 HD1 TRP A 38152.207 10.086 4.378 1.00 0.00 H ATOM 532 HE1 TRP A 38152.794 11.659 2.426 1.00 0.00 H **ATOM** 533 HE3 TRP A 38151.849 6.756 0.517 1.00 0.00 H **ATOM** 534 HZ2 TRP A 38153.065 11.506 -0.381 1.00 0.00 H **ATOM** 535 HZ3 TRP A 38152.290 7.547 -1.770 1.00 0.00 H **ATOM** 536 HH2 TRP A 38152.887 9.873 -2.209 1.00 0.00 H **ATOM** 537 N ILE A 39148.781 8.499 2.204 1.00 0.00 N **ATOM** 538 CA ILE A 39148.111 8.845 0.957 1.00 0.00 C ATOM 539 C ILE A 39148.616 10.185 0.433 1.00 0.00 C **ATOM** 540 O ILE A 39148.281 11.239 0.974 1.00 0.00 O **ATOM** 541 CB ILE A 39146.583 8.917 1.137 1.00 0.00 C **ATOM** 542 CG1 ILE A 39146.066 7.647 1.816 1.00 0.00 C **ATOM** 543 CG2 ILE A 39145.898 9.121 -0.206 1.00 0.00 C **ATOM** 544 CD1 ILE A 39144.781 7.854 2.588 1.00 0.00 C **ATOM** 545 H ILE A 39148.726 9.117 2.963 1.00 0.00 H **ATOM** 546 HA ILE A 39148.335 8.077 0.231 1.00 0.00 H **ATOM** 547 HB ILE A 39146.356 9.767 1.761 1.00 0.00 H ATOM 548 1HG1 ILE A 39145.881 6.894 1.064 1.00 0.00 H **ATOM** 549 2HG1 ILE A 39146.814 7.285 2.506 1.00 0.00 H ATOM 550 1HG2 ILE A 39146.213 8.348 -0.892 1.00 0.00 H **ATOM** ATOM 551 2HG2 ILE A 39146.169 10.088 -0.605 1.00 0.00 H

552 3HG2 ILE A 39144.827 9.073 -0.076 1.00 0.00 H ATOM 553 1HD1 ILE A 39144.535 6.952 3.127 1.00 0.00 H **ATOM ATOM** 554 2HD1 ILE A 39143.983 8.092 1.900 1.00 0.00 H 555 3HD1 ILE A 39144.908 8.668 3.286 1.00 0.00 H ATOM 556 N GLY A 40149.429 10.140 -0.617 1.00 0.00 N **ATOM** 557 CA GLY A 40149.970 11.360 -1.185 1.00 0.00 C ATOM **ATOM** 558 C GLYA 40150.570 11.152 -2.561 1.00 0.00 C 559 O GLY A 40150.382 10.103 -3.177 1.00 0.00 O **ATOM** 560 H GLY A 40149.667 9.272 -1.006 1.00 0.00 H ATOM 561 1HA GLY A 40149.179 12.091 -1.257 1.00 0.00 H **ATOM** 562 2HA GLY A 40150.735 11.740 -0.525 1.00 0.00 H ATOM 563 N GLNA 41151.290 12.159 -3.044 1.00 0.00 N ATOM 564 CA GLN A 41151.919 12.094 -4.355 1.00 0.00 C ATOM 565 C GLN A 41153.396 12.478 -4.267 1.00 0.00 C ATOM 566 O GLN A 41153.728 13.616 -3.935 1.00 0.00 O ATOM 567 CB GLN A 41151.195 13.024 -5.325 1.00 0.00 C **ATOM** 568 CG GLN A 41149.683 12.862 -5.309 1.00 0.00 C ATOM 569 CD GLN A 41148.955 14.188 -5.405 1.00 0.00 C **ATOM** 570 OE1 GLN A 41148.905 14.953 -4.443 1.00 0.00 O ATOM 571 NE2 GLN A 41148.387 14.464 -6.571 1.00 0.00 N **ATOM** 572 H GLN A 41151.398 12.969 -2.505 1.00 0.00 H **ATOM** 573 HA GLN A 41151.839 11.080 -4.713 1.00 0.00 H **ATOM** 574 1HB GLN A 41151.427 14.046 -5.067 1.00 0.00 H **ATOM** 575 2HB GLN A 41151.546 12.826 -6.325 1.00 0.00 H ATOM 576 1HG GLN A 41149.390 12.247 -6.145 1.00 0.00 H ATOM 577 2HG GLN A 41149.396 12.376 -4.388 1.00 0.00 H ATOM 578 1HE2 GLN A 41148.468 13.805 -7.292 1.00 0.00 H **ATOM** 579 2HE2 GLN A 41147.910 15.314 -6.665 1.00 0.00 H ATOM 580 N PRO A 42154.309 11.532 -4.559 1.00 0.00 N **ATOM** 581 CA PRO A 42155.752 11.787 -4.505 1.00 0.00 C ATOM 582 C PRO A 42156.172 12.938 -5.414 1.00 0.00 C

583 O PROA 42155.454 13.294 -6.350 1.00 0.00 O **ATOM** 584 CB PRO A 42156.371 10.471 -4.989 1.00 0.00 C ATOM 585 CG PRO A 42155.320 9.444 -4.752 1.00 0.00 C ATOM 586 CD PRO A 42154.010 10.147 -4.961 1.00 0.00 C 587 HA PRO A 42156.079 11.991 -3.496 1.00 0.00 H **ATOM** 588 1HB PRO A 42156.616 10.552 -6.039 1.00 0.00 H **ATOM** ATOM 589 2HB PRO A 42157.265 10.260 -4.420 1.00 0.00 H 590 1HG PRO A 42155.429 8.634 -5.458 1.00 0.00 H **ATOM ATOM** 591 2HG PRO A 42155.389 9.074 -3.739 1.00 0.00 H 592 1HD PRO A 42153.719 10.100 -6.000 1.00 0.00 H **ATOM** 593 2HD PRO A 42153.244 9.717 -4.331 1.00 0.00 H **ATOM** 594 N PRO A 43157.345 13.537 -5.151 1.00 0.00 N **ATOM** 595 CA PRO A 43157.858 14.653 -5.950 1.00 0.00 C **ATOM** 596 C PRO A 43158.331 14.206 -7.328 1.00 0.00 C ATOM 597 O PRO A 43159.507 13.894 -7.520 1.00 0.00 O **ATOM** 598 CB PRO A 43159.035 15.169 -5.124 1.00 0.00 C ATOM 599 CG PRO A 43159.493 13.989 -4.340 1.00 0.00 C ATOM ATOM 600 CD PRO A 43158.261 13.173 -4.054 1.00 0.00 C 601 HA PRO A 43157.120 15.433 -6.060 1.00 0.00 H ATOM 602 1HB PRO A 43159.809 15.530 -5.785 1.00 0.00 H ATOM 603 2HB PRO A 43158.703 15.968 -4.478 1.00 0.00 H ATOM 604 1HG PRO A 43160.198 13.412 -4.922 1.00 0.00 H ATOM 605 2HG PRO A 43159.948 14.316 -3.417 1.00 0.00 H **ATOM ATOM** 606 1HD PRO A 43158.493 12.119 -4.080 1.00 0.00 H 607 2HD PRO A 43157.843 13.445 -3.096 1.00 0.00 H ATOM 608 N GLY A 44157.411 14.178 -8.286 1.00 0.00 N **ATOM** 609 CA GLY A 44157.758 13.769 -9.633 1.00 0.00 C ATOM 610 C GLY A 44156.560 13.280 -10.418 1.00 0.00 C ATOM 611 O GLY A 44156.327 13.716 -11.546 1.00 0.00 O ATOM 612 H GLYA 44156.490 14.438 -8.076 1.00 0.00 H **ATOM** ATOM 613 1HA GLY A 44158.194 14.610 -10.151 1.00 0.00 H

614 2HA GLY A 44158.488 12.976 -9.579 1.00 0.00 H 615 N LEUA 45155.794 12.370 -9.824 1.00 0.00 N ATOM 616 CA LEU A 45154.613 11.822 -10.479 1.00 0.00 C **ATOM** ATOM 617 C LEUA 45153.363 12.082 -9.648 1.00 0.00 C 618 O LEUA 45153.203 11.525 -8.562 1.00 0.00 O ATOM 619 CB LEU A 45154.783 10.318 -10.708 1.00 0.00 C ATOM 620 CG LEU A 45155.251 9.525 -9.486 1.00 0.00 C ATOM 621 CD1 LEU A 45154.856 8.060 -9.614 1.00 0.00 C ATOM 622 CD2 LEU A 45156.757 9.664 -9.304 1.00 0.00 C **ATOM** 623 H LEUA 45156.030 12.060 -8.922 1.00 0.00 H **ATOM** 624 HA LEU A 45154.505 12.313 -11.435 1.00 0.00 H ATOM 625 1HB LEU A 45153.834 9.915 -11.032 1.00 0.00 H ATOM **ATOM** 626 2HB LEU A 45155.504 10.175 -11.499 1.00 0.00 H 627 HG LEU A 45154.770 9.923 -8.604 1.00 0.00 H ATOM 628 1HD1 LEU A 45154.124 7.818 -8.858 1.00 0.00 H **ATOM** 629 2HD1 LEU A 45155.729 7.438 -9.480 1.00 0.00 H **ATOM** 630 3HD1 LEU A 45154.437 7.883 -10.593 1.00 0.00 H **ATOM** 631 1HD2 LEU A 45156.974 9.910 -8.275 1.00 0.00 H ATOM 632 2HD2 LEU A 45157.127 10.451 -9.947 1.00 0.00 H ATOM 633 3HD2 LEU A 45157.239 8.733 -9.562 1.00 0.00 H ATOM 634 N ASN A 46152.477 12.930 -10.162 1.00 0.00 N ATOM 635 CA ASN A 46151.245 13.251 -9.454 1.00 0.00 C ATOM 636 C ASN A 46150.273 12.078 -9.511 1.00 0.00 C **ATOM** 637 O ASN A 46149.690 11.790 -10.556 1.00 0.00 O **ATOM** 638 CB ASN A 46150.597 14.498 -10.061 1.00 0.00 C ATOM 639 CG ASN A 46149.341 14.917 -9.325 1.00 0.00 C ATOM 640 OD1 ASN A 46149.358 15.856 -8.529 1.00 0.00 O ATOM 641 ND2 ASN A 46148.241 14.221 -9.587 1.00 0.00 N **ATOM** 642 H ASN A 46152.654 13.344 -11.032 1.00 0.00 H ATOM 643 HA ASN A 46151.494 13.450 -8.423 1.00 0.00 H ATOM ATOM 644 1HB ASN A 46151.301 15.315 -10.025 1.00 0.00 H

645 2HB ASN A 46150.338 14.296 -11.091 1.00 0.00 H **ATOM** 646 1HD2 ASN A 46148.301 13.486 -10.233 1.00 0.00 H **ATOM** 647 2HD2 ASN A 46147.413 14.471 -9.125 1.00 0.00 H **ATOM** 648 N GLUA 47150.105 11.406 -8.378 1.00 0.00 N **ATOM** 649 CA GLUA 47149.205 10.262 -8.289 1.00 0.00 C ATOM **ATOM** 650 C GLUA 47148.956 9.884 -6.833 1.00 0.00 C 651 O GLUA 47149.896 9.621 -6.083 1.00 0.00 O ATOM 652 CB GLU A 47149.782 9.066 -9.049 1.00 0.00 C ATOM 653 CG GLU A 47151.289 8.916 -8.907 1.00 0.00 C ATOM 654 CD GLU Á 47151.881 7.979 -9.941 1.00 0.00 C **ATOM** 655 OE1 GLU A 47152.122 8.429 -11.081 1.00 0.00 O **ATOM** 656 OE2 GLU A 47152.104 6.795 -9.612 1.00 0.00 O **ATOM** 657 H GLUA 47150.599 11.686 -7.580 1.00 0.00 H **ATOM** 658 HA GLU A 47148.266 10.545 -8.740 1.00 0.00 H ATOM 659 1HB GLU A 47149.317 8.163 -8.682 1.00 0.00 H ATOM 660 2HB GLU A 47149.550 9.176 -10.099 1.00 0.00 H ATOM 661 1HG GLU A 47151.746 9.887 -9.021 1.00 0.00 H **ATOM** 662 2HG GLU A 47151.509 8.529 -7.924 1.00 0.00 H ATOM 663 N VALA 48147.688 9.850 -6.439 1.00 0.00 N ATOM 664 CA VALA 48147.331 9.494 -5.072 1.00 0.00 C **ATOM** 665 C VALA 48147.655 8.030 -4.795 1.00 0.00 C **ATOM** 666 O VALA 48146.912 7.133 -5.191 1.00 0.00 O **ATOM** 667 CB VAL A 48145.835 9.739 -4.796 1.00 0.00 C **ATOM** 668 CG1 VAL A 48145.527 9.554 -3.319 1.00 0.00 C ATOM 669 CG2 VAL A 48145.427 11.128 -5.265 1.00 0.00 C **ATOM** 670 H VALA 48146.979 10.064 -7.080 1.00 0.00 H **ATOM** 671 HA VALA 48147.908 10.113 -4.401 1.00 0.00 H ATOM 672 HB VALA 48145.263 9.012 -5.353 1.00 0.00 H **ATOM** 673 1HG1 VAL A 48145.685 8.522 -3.044 1.00 0.00 H ATOM 674 2HG1 VAL A 48144.498 9.824 -3.129 1.00 0.00 H ATOM

675 3HG1 VAL A 48146.178 10.186 -2.733 1.00 0.00 H

676 1HG2 VAL A 48145.171 11.092 -6.314 1.00 0.00 H 677 2HG2 VAL A 48146.248 11.813 -5.118 1.00 0.00 H **ATOM** 678 3HG2 VAL A 48144.572 11.462 -4.697 1.00 0.00 H ATOM 679 N LEUA 49148.771 7.795 -4.114 1.00 0.00 N **ATOM** 680 CA LEUA 49149.196 6.439 -3.787 1.00 0.00 C **ATOM** 681 C LEUA 49149.018 6.158 -2.301 1.00 0.00 C ATOM 682 O LEUA 49149.659 6.789 -1.460 1.00 0.00 O **ATOM** 683 CB LEU A 49150.657 6.228 -4.185 1.00 0.00 C **ATOM** 684 CG LEUA 49150.989 6.568 -5.640 1.00 0.00 C **ATOM** 685 CD1 LEU A 49152.472 6.871 -5.792 1.00 0.00 C **ATOM** 686 CD2 LEU A 49150.580 5.427 -6.559 1.00 0.00 C **ATOM** 687 H LEUA 49149.325 8.551 -3.824 1.00 0.00 H **ATOM** 688 HA LEUA 49148.577 5.754 -4.347 1.00 0.00 H **ATOM** 689 1HB LEU A 49151.275 6.841 -3.544 1.00 0.00 H **ATOM** 690 2HB LEU A 49150.909 5.192 -4.016 1.00 0.00 H **ATOM** 691 HG LEUA 49150.437 7.449 -5.931 1.00 0.00 H **ATOM** 692 1HD1 LEU A 49152.882 7.153 -4.833 1.00 0.00 H ATOM 693 2HD1 LEU A 49152.604 7.682 -6.492 1.00 0.00 H ATOM 694 3HD1 LEU A 49152.984 5.993 -6.157 1.00 0.00 H **ATOM** 695 1HD2 LEU A 49149.667 4.980 -6.195 1.00 0.00 H **ATOM ATOM** 696 2HD2 LEU A 49151.362 4.682 -6.578 1.00 0.00 H 697 3HD2 LEU A 49150.421 5.808 -7.556 1.00 0.00 H ATOM 698 N ALAA 50148.145 5.210 -1.983 1.00 0.00 N ATOM 699 CA ALAA 50147.887 4.849 -0.596 1.00 0.00 C ATOM 700 C ALAA 50148.794 3.707 -0.151 1.00 0.00 C **ATOM** 701 O ALAA 50148.698 2.591 -0.660 1.00 0.00 O ATOM 702 CB ALAA 50146.426 4.471 -0.412 1.00 0.00 C ATOM 703 H ALAA 50147.665 4.741 -2.698 1.00 0.00 H **ATOM** 704 HA ALAA 50148.091 5.718 0.013 1.00 0.00 H **ATOM** 705 1HB ALAA 50146.071 4.857 0.531 1.00 0.00 H **ATOM** 706 2HB ALA A 50146.329 3.395 -0.421 1.00 0.00 H ATOM

707 3HB ALAA 50145.841 4.890 -1.217 1.00 0.00 H **ATOM** 708 N GLYA 51149.675 3.995 0.801 1.00 0.00 N **ATOM** 709 CA GLY A 51150.587 2.981 1.299 1.00 0.00 C **ATOM** 710 C GLY A 51149.892 1.946 2.160 1.00 0.00 C **ATOM** 711 O GLYA 51149.589 2.200 3.325 1.00 0.00 O **ATOM** 712 H GLY A 51149.707 4.902 1.170 1.00 0.00 H **ATOM ATOM** 713 1HA GLY A 51151.047 2.483 0.458 1.00 0.00 H 714 2HA GLY A 51151.356 3.462 1.885 1.00 0.00 H **ATOM** 715 N LEUA 52149.638 0.775 1.585 1.00 0.00 N **ATOM** 716 CA LEUA 52148.973 -0.303 2.309 1.00 0.00 C **ATOM** 717 C LEUA 52149.989 -1.169 3.048 1.00 0.00 C **ATOM ATOM** 718 O LEUA 52151.096 -1.398 2.561 1.00 0.00 O 719 CB LEUA 52148.157 -1.166 1.345 1.00 0.00 C **ATOM** 720 CG LEU A 52146.971 -0.456 0.688 1.00 0.00 C **ATOM** 721 CD1 LEU A 52146.473 -1.249 -0.511 1.00 0.00 C **ATOM ATOM** 722 CD2 LEU A 52145.850 -0.249 1.695 1.00 0.00 C **ATOM** 723 H LEUA 52149.904 0.632 0.653 1.00 0.00 H 724 HA LEU A 52148.307 0.145 3.030 1.00 0.00 H **ATOM** 725 1HB LEU A 52148.816 -1.520 0.565 1.00 0.00 H **ATOM ATOM** 726 2HB LEU A 52147.780 -2.018 1.889 1.00 0.00 H 727 HG LEU A 52147.291 0.514 0.337 1.00 0.00 H **ATOM ATOM** 728 1HD1 LEU A 52147.292 -1.809 -0.937 1.00 0.00 H 729 2HD1 LEU A 52146.077 -0.569 -1.252 1.00 0.00 H **ATOM** 730 3HD1 LEU A 52145.696 -1.929 -0.195 1.00 0.00 H **ATOM** 731 1HD2 LEU A 52145.336 -1.185 1.860 1.00 0.00 H ATOM 732 2HD2 LEU A 52145.154 0.482 1.314 1.00 0.00 H ATOM 733 3HD2 LEU A 52146.266 0.102 2.628 1.00 0.00 H ATOM **ATOM** 734 N GLUA 53149.603 -1.646 4.227 1.00 0.00 N 735 CA GLU A 53150.479 -2.487 5.035 1.00 0.00 C ATOM 736 C GLUA 53149.945 -3.914 5.110 1.00 0.00 C **ATOM** 737 O GLUA 53148.905 -4.167 5.719 1.00 0.00 O ATOM

738 CB GLU A 53150.619 -1.908 6.444 1.00 0.00 C **ATOM** 739 CG GLU A 53151.548 -2.709 7.342 1.00 0.00 C **ATOM** 740 CD GLU A 53151.003 -2.872 8.747 1.00 0.00 C **ATOM ATOM** 741 OE1 GLU A 53150.405 -3.929 9.034 1.00 0.00 O 742 OE2 GLU A 53151.176 -1.940 9.563 1.00 0.00 O **ATOM** 743 H GLUA 53148.708 -1.428 4.562 1.00 0.00 H **ATOM** 744 HA GLU A 53151.451 -2.503 4.564 1.00 0.00 H ATOM 745 1HB GLU A 53151.004 -0.902 6.370 1.00 0.00 H **ATOM** 746 2HB GLU A 53149.644 -1.877 6.907 1.00 0.00 H ATOM 747 1HG GLUA 53151.686 -3.690 6.911 1.00 0.00 H **ATOM** 748 2HG GLU A 53152.500 -2.203 7.396 1.00 0.00 H **ATOM** 749 N LEUA 54150.663 -4.842 4.488 1.00 0.00 N ATOM **ATOM** 750 CA LEU A 54150.262 -6.244 4.484 1.00 0.00 C 751 C LEU A 54150.392 -6.851 5.878 1.00 0.00 C ATOM 752 O LEUA 54151.214 -6.411 6.682 1.00 0.00 O **ATOM** 753 CB LEU A 54151.110 -7.037 3.488 1.00 0.00 C **ATOM** 754 CG LEUA 54151.206 -6.425 2.090 1.00 0.00 C **ATOM** 755 CD1 LEU A 54152.397 -6.999 1.338 1.00 0.00 C **ATOM** 756 CD2 LEU A 54149.919 -6.664 1.315 1.00 0.00 C **ATOM** 757 H LEUA 54151.483 -4.580 4.020 1.00 0.00 H **ATOM** 758 HA LEUA 54149.227 -6.292 4.180 1.00 0.00 H **ATOM** 759 1HB LEU A 54152.108 -7.127 3.890 1.00 0.00 H **ATOM** 760 2HB LEU A 54150.687 -8.026 3.396 1.00 0.00 H **ATOM ATOM** 761 HG LEU A 54151.352 -5.358 2.180 1.00 0.00 H 762 1HD1 LEU A 54152.143 -7.976 0.952 1.00 0.00 H ATOM 763 2HD1 LEU A 54153.239 -7.086 2.009 1.00 0.00 H **ATOM** 764 3HD1 LEU A 54152.656 -6.345 0.519 1.00 0.00 H ATOM 765 1HD2 LEU A 54149.250 -5.828 1.463 1.00 0.00 H **ATOM** 766 2HD2 LEU A 54149.448 -7.569 1.667 1.00 0.00 H ATOM 767 3HD2 LEU A 54150.145 -6.761 0.263 1.00 0.00 H **ATOM** 768 N GLUA 55149.577 -7.864 6.156 1.00 0.00 N ATOM

769 CA GLUA 55149.603 -8.531 7.451 1.00 0.00 C ATOM 770 C GLUA 55150.652 -9.638 7.472 1.00 0.00 C **ATOM** 771 O GLUA 55151.247 -9.925 8.511 1.00 0.00 O **ATOM** 772 CB GLU A 55148.225 -9.112 7.777 1.00 0.00 C ATOM 773 CG GLUA 55147.239 -8.081 8.300 1.00 0.00 C ATOM 774 CD GLUA 55147.170 -8.058 9.815 1.00 0.00 C **ATOM** 775 OE1 GLU A 55146.195 -8.603 10.374 1.00 0.00 O **ATOM** 776 OE2 GLU A 55148.091 -7.495 10.444 1.00 0.00 O **ATOM** 777 H GLUA 55148.945 -8.169 5.473 1.00 0.00 H ATOM 778 HA GLU A 55149.859 -7.795 8.199 1.00 0.00 H **ATOM** 779 1HB GLU A 55147.812 -9.551 6.880 1.00 0.00 H **ATOM** 780 2HB GLU A 55148.339 -9.882 8.525 1.00 0.00 H **ATOM** 781 1HG GLU A 55147.543 -7.103 7.955 1.00 0.00 H **ATOM** 782 2HG GLU A 55146.258 -8.311 7.913 1.00 0.00 H **ATOM** 783 N ASPA 56150.874 -10.258 6.317 1.00 0.00 N **ATOM** 784 CA ASPA 56151.851 -11.333 6.202 1.00 0.00 C **ATOM** 785 C ASPA 56153.173 -10.811 5.649 1.00 0.00 C **ATOM** 786 O ASPA 56153.208 -10.169 4.599 1.00 0.00 O **ATOM** 787 CB ASP A 56151.313 -12.446 5.301 1.00 0.00 C **ATOM** 788 CG ASP A 56150.352 -13.365 6.029 1.00 0.00 C ATOM 789 OD1 ASP A 56149.236 -13.588 5.512 1.00 0.00 O **ATOM** 790 OD2 ASP A 56150.715 -13.864 7.114 1.00 0.00 O **ATOM** 791 H ASPA 56150.368 -9.984 5.523 1.00 0.00 H **ATOM** 792 HA ASP A 56152.022 -11.733 7.190 1.00 0.00 H **ATOM** 793 1HB ASP A 56150.793 -12.004 4.464 1.00 0.00 H **ATOM** 794 2HB ASP A 56152.140 -13.036 4.934 1.00 0.00 H ATOM 795 N GLUA 57154.259 -11.088 6.363 1.00 0.00 N **ATOM** 796 CA GLU A 57155.584 -10.645 5.943 1.00 0.00 C ATOM 797 C GLUA 57156.033 -11.387 4.689 1.00 0.00 C **ATOM** 798 O GLUA 57156.555 -12.499 4.766 1.00 0.00 O **ATOM** 799 CB GLU A 57156.597 -10.862 7.068 1.00 0.00 C ATOM

800 CG GLUA 57156.634 -9.728 8.079 1.00 0.00 C 801 CD GLUA 57157.934 -9.686 8.859 1.00 0.00 C **ATOM** 802 OE1 GLU A 57158.886 -9.025 8.391 1.00 0.00 O **ATOM** 803 OE2 GLU A 57158.001 -10.312 9.938 1.00 0.00 O **ATOM** ATOM 804 H GLUA 57154.167 -11.603 7.192 1.00 0.00 H **ATOM** 805 HA GLU A 57155.525 -9.590 5.722 1.00 0.00 H 806 1HB GLU A 57156.348 -11.774 7.591 1.00 0.00 H ATOM 807 2HB GLU A 57157.582 -10.963 6.636 1.00 0.00 H **ATOM** 808 1HG GLUA 57156.517 -8.792 7.557 1.00 0.00 H **ATOM ATOM** 809 2HG GLU A 57155.819 -9.856 8.776 1.00 0.00 H 810 N CYS A 58155.825 -10.764 3.533 1.00 0.00 N ATOM 811 CA CYS A 58156.210 -11.364 2.261 1.00 0.00 C ATOM 812 C CYS A 58157.455 -10.689 1.695 1.00 0.00 C ATOM 813 O CYS A 58157.512 -9.465 1.580 1.00 0.00 O **ATOM ATOM** 814 CB CYS A 58155.060 -11.263 1.258 1.00 0.00 C 815 SG CYS A 58155.200 -12.400 -0.142 1.00 0.00 S **ATOM** 816 H CYS A 58155.405 -9.879 3.536 1.00 0.00 H **ATOM** 817 HA CYS A 58156.429 -12.406 2.440 1.00 0.00 H **ATOM ATOM** 818 1HB CYS A 58154.131 -11.480 1.763 1.00 0.00 H 819 2HB CYS A 58155.023 -10.257 0.864 1.00 0.00 H **ATOM** 820 HG CYS A 58155.346 -13.282 0.206 1.00 0.00 H **ATOM** 821 N ALAA 59158.450 -11.497 1.343 1.00 0.00 N **ATOM** 822 CA ALAA 59159.695 -10.978 0.787 1.00 0.00 C ATOM 823 C ALA A 59159.453 -10.283 -0.548 1.00 0.00 C ATOM 824 O ALAA 59158.956 -10.893 -1.495 1.00 0.00 O **ATOM** 825 CB ALAA 59160.709 -12.100 0.625 1.00 0.00 C ATOM 826 H ALAA 59158.345 -12.464 1.458 1.00 0.00 H **ATOM** 827 HA ALAA 59160.097 -10.259 1.487 1.00 0.00 H ATOM 828 1HB ALAA 59161.226 -12.256 1.561 1.00 0.00 H **ATOM** 829 2HB ALAA 59161.421 -11.833 -0.141 1.00 0.00 H ATOM ATOM 830 3HB ALA A 59160.197 -13.008 0.341 1.00 0.00 H

- 831 N GLYA 60159.808 -9.005 -0.618 1.00 0.00 N 832 CA GLY A 60159.622 -8.249 -1.842 1.00 0.00 C ATOM 833 C GLY A 60159.105 -6.847 -1.587 1.00 0.00 C **ATOM** 834 O GLY A 60159.364 -5.931 -2.367 1.00 0.00 O ATOM ATOM 835 H GLY A 60160.200 -8.570 0.169 1.00 0.00 H ATOM 836 1HA GLY A 60160.568 -8.184 -2.359 1.00 0.00 H 837 2HA GLY A 60158.916 -8.772 -2.471 1.00 0.00 H **ATOM** 838 N CYS A 61158.372 -6.679 -0.491 1.00 0.00 N ATOM 839 CA CYS A 61157.818 -5.378 -0.135 1.00 0.00 C **ATOM** 840 C CYS A 61158.817 -4.564 0.680 1.00 0.00 C **ATOM** 841 O CYS A 61159.828 -5.091 1.147 1.00 0.00 O ATOM 842 CB CYS A 61156.519 -5.553 0.656 1.00 0.00 C ATOM 843 SG CYS A 61155.273 -6.557 -0.185 1.00 0.00 S ATOM 844 H CYS A 61158.200 -7.447 0.092 1.00 0.00 H ATOM ATOM 845 HA CYS A 61157.602 -4.848 -1.050 1.00 0.00 H 846 1HB CYS A 61156.742 -6.029 1.598 1.00 0.00 H ATOM 847 2HB CYS A 61156.087 -4.581 0.843 1.00 0.00 H **ATOM** 848 HG CYS A 61154.755 -7.009 0.485 1.00 0.00 H ATOM 849 N THR A 62158.529 -3.278 0.848 1.00 0.00 N ATOM 850 CA THR A 62159.402 -2.391 1.608 1.00 0.00 C ATOM 851 C THR A 62158.917 -2.249 3.047 1.00 0.00 C ATOM 852 O THR A 62157.942 -2.885 3.448 1.00 0.00 O ATOM
- 853 CB THR A 62159.471 -1.016 0.942 1.00 0.00 C **ATOM**
- 854 OG1 THR A 62158.253 -0.718 0.283 1.00 0.00 O ATOM
- 855 CG2 THR A 62160.584 -0.898 -0.076 1.00 0.00 C ATOM
- 856 H THR A 62157.709 -2.916 0.453 1.00 0.00 H ATOM
- ATOM 857 HA THR A 62160.390 -2.827 1.616 1.00 0.00 H
- 858 HB THR A 62159.637 -0.267 1.703 1.00 0.00 H ATOM
- 859 HG1 THR A 62158.243 0.209 0.033 1.00 0.00 H ATOM
- ATOM 860 1HG2 THR A 62161.538 -0.993 0.421 1.00 0.00 H
- 861 2HG2 THR A 62160.526 0.064 -0.563 1.00 0.00 H ATOM

ATOM 862 3HG2 THR A 62160.483 -1.681 -0.812 1.00 0.00 H

ATOM 863 N ASPA 63159.602 -1.412 3.818 1.00 0.00 N

ATOM 864 CA ASP A 63159.240 -1.185 5.212 1.00 0.00 C

ATOM 865 C ASPA 63158.612 0.192 5.394 1.00 0.00 C

ATOM 866 O ASPA 63158.751 0.814 6.448 1.00 0.00 O

ATOM 867 CB ASP A 63160.473 -1.319 6.108 1.00 0.00 C

ATOM 868 CG ASP A 63161.586 -0.372 5.706 1.00 0.00 C

ATOM 869 OD1 ASP A 63162.107 -0.513 4.580 1.00 0.00 O

ATOM 870 OD2 ASP A 63161.935 0.512 6.517 1.00 0.00 O

ATOM 871 H ASPA 63160.370 -0.933 3.440 1.00 0.00 H

ATOM 872 HA ASP A 63158.518 -1.938 5.493 1.00 0.00 H

ATOM 873 1HB ASP A 63160.193 -1.104 7.129 1.00 0.00 H

ATOM 874 2HB ASP A 63160.846 -2.331 6.048 1.00 0.00 H

ATOM 875 N GLY A 64157.919 0.662 4.363 1.00 0.00 N

ATOM 876 CA GLY A 64157.278 1.963 4.429 1.00 0.00 C

ATOM 877 C GLY A 64158.053 3.031 3.681 1.00 0.00 C

ATOM 878 O GLY A 64158.129 4.177 4.125 1.00 0.00 O

ATOM 879 H GLY A 64157.841 0.122 3.548 1.00 0.00 H

ATOM 880 1HA GLY A 64156.289 1.887 4.004 1.00 0.00 H

ATOM 881 2HA GLY A 64157.192 2.256 5.466 1.00 0.00 H

ATOM 882 N THR A 65158.628 2.654 2.544 1.00 0.00 N

ATOM 883 CA THR A 65159.401 3.587 1.733 1.00 0.00 C

ATOM 884 C THR A 65159.066 3.428 0.253 1.00 0.00 C

ATOM 885 O THR A 65159.267 2.360 -0.328 1.00 0.00 O

ATOM 886 CB THR A 65160.898 3.371 1.955 1.00 0.00 C

ATOM 887 OG1 THR A 65161.198 1.990 2.046 1.00 0.00 O

ATOM 888 CG2 THR A 65161.419 4.037 3.210 1.00 0.00 C

ATOM 889 H THR A 65158.532 1.726 2.243 1.00 0.00 H

ATOM 890 HA THR A 65159.141 4.589 2.042 1.00 0.00 H

ATOM 891 HB THR A 65161.439 3.780 1.113 1.00 0.00 H

ATOM 892 HG1 THR A 65160.877 1.539 1.261 1.00 0.00 H

893 1HG2 THR A 65161.665 5.067 2.995 1.00 0.00 H ATOM **ATOM** 894 2HG2 THR A 65162.303 3.520 3.551 1.00 0.00 H 895 3HG2 THR A 65160.661 4.001 3.978 1.00 0.00 H ATOM 896 N PHE A 66158.556 4.496 -0.352 1.00 0.00 N **ATOM** 897 CA PHE A 66158.193 4.473 -1.764 1.00 0.00 C **ATOM** 898 C PHE A 66159.281 5.122 -2.615 1.00 0.00 C **ATOM** 899 O PHE A 66159,440 6.343 -2.613 1.00 0.00 O ATOM **ATOM** 900 CB PHE A 66156.862 5.195 -1.982 1.00 0.00 C 901 CG PHE A 66156.296 5.008 -3.360 1.00 0.00 C **ATOM** 902 CD1 PHE A 66155.867 3.760 -3.784 1.00 0.00 C **ATOM** 903 CD2 PHE A 66156.194 6.080 -4.233 1.00 0.00 C **ATOM** 904 CE1 PHE A 66155.346 3.585 -5.052 1.00 0.00 C **ATOM** 905 CE2 PHE A 66155.674 5.910 -5.502 1.00 0.00 C **ATOM** 906 CZ PHE A 66155.249 4.662 -5.912 1.00 0.00 C **ATOM** 907 H PHE A 66158.419 5.317 0.164 1.00 0.00 H **ATOM** 908 HA PHE A 66158.086 3.442 -2.063 1.00 0.00 H ATOM 909 1HB PHE A 66156.138 4.821 -1.272 1.00 0.00 H **ATOM** ATOM 910 2HB PHE A 66157.004 6.254 -1.820 1.00 0.00 H 911 HD1 PHE A 66155.942 2.918 -3.112 1.00 0.00 H **ATOM** 912 HD2 PHE A 66156.525 7.056 -3.913 1.00 0.00 H **ATOM** 913 HE1 PHE A 66155.016 2.608 -5.371 1.00 0.00 H **ATOM** 914 HE2 PHE A 66155.599 6.754 -6.172 1.00 0.00 H ATOM 915 HZ PHE A 66154.843 4.527 -6.904 1.00 0.00 H **ATOM** 916 N ARG A 67160.027 4.296 -3.341 1.00 0.00 N **ATOM** 917 CA ARG A 67161.100 4.789 -4.198 1.00 0.00 C **ATOM** 918 C ARG A 67162.157 5.521 -3.378 1.00 0.00 C **ATOM** 919 O ARG A 67162.675 6.557 -3.798 1.00 0.00 O ATOM 920 CB ARG A 67160.534 5.719 -5.274 1.00 0.00 C **ATOM** 921 CG ARG A 67159.459 5.073 -6.133 1.00 0.00 C ATOM 922 CD ARG A 67159.356 5.744 -7.493 1.00 0.00 C ATOM ATOM 923 NE ARG A 67159.127 4.777 -8.564 1.00 0.00 N

924 CZ ARG A 67159.155 5.084 -9.859 1.00 0.00 C 925 NH1 ARG A 67159.400 6.331 -10.247 1.00 0.00 N ATOM 926 NH2 ARG A 67158.938 4.145 -10.769 1.00 0.00 N ATOM ATOM 927 H ARG A 67159.851 3.333 -3.302 1.00 0.00 H ATOM 928 HA ARG A 67161.559 3.937 -4.677 1.00 0.00 H ATOM 929 1HB ARG A 67160.107 6.587 -4.794 1.00 0.00 H 930 2HB ARG A 67161.340 6.035 -5.920 1.00 0.00 H ATOM **ATOM** 931 1HG ARG A 67159.705 4.031 -6.275 1.00 0.00 H **ATOM** 932 2HG ARG A 67158.509 5.156 -5.626 1.00 0.00 H 933 1HD ARG A 67158.534 6.444 -7.473 1.00 0.00 H **ATOM** 934 2HD ARG A 67160.275 6.275 -7.690 1.00 0.00 H ATOM 935 HE ARG A 67158.944 3.850 -8.305 1.00 0.00 H **ATOM** ATOM 936 1HH1 ARG A 67159.565 7.044 -9.566 1.00 0.00 H **ATOM** 937 2HH1 ARG A 67159.421 6.555 -11.221 1.00 0.00 H **ATOM** 938 1HH2 ARG A 67158.753 3.205 -10.481 1.00 0.00 H **ATOM** 939 2HH2 ARG A 67158.958 4.375 -11.741 1.00 0.00 H 940 N GLY A 68162.473 4.977 -2.208 1.00 0.00 N **ATOM** 941 CA GLY A 68163.468 5.592 -1.349 1.00 0.00 C ATOM 942 C GLY A 68162.935 6.814 -0.627 1.00 0.00 C ATOM ATOM 943 O GLY A 68163.691 7.728 -0.297 1.00 0.00 O 944 H GLY A 68162.027 4.152 -1.926 1.00 0.00 H ATOM 945 1HA GLY A 68163.792 4.868 -0.617 1.00 0.00 H **ATOM** 946 2HA GLY A 68164.315 5.885 -1.950 1.00 0.00 H **ATOM** ATOM 947 N THR A 69161.629 6.830 -0.382 1.00 0.00 N **ATOM** 948 CA THR A 69160.994 7.950 0.305 1.00 0.00 C 949 C THR A 69160.067 7.454 1.411 1.00 0.00 C ATOM 950 O THR A 69158.900 7.147 1.164 1.00 0.00 O **ATOM** 951 CB THR A 69160.209 8.807 -0.689 1.00 0.00 C ATOM 952 OG1 THR A 69160.975 9.048 -1.855 1.00 0.00 O ATOM **ATOM** 953 CG2 THR A 69159.796 10.148 -0.125 1.00 0.00 C ATOM 954 H THR A 69161.078 6.073 -0.669 1.00 0.00 H

955 HA THR A 69161.774 8.551 0.749 1.00 0.00 H ATOM 956 HB THR A 69159.312 8.277 -0.974 1.00 0.00 H ATOM 957 HG1 THR A 69160.699 8.445 -2.550 1.00 0.00 H **ATOM ATOM** 958 1HG2 THR A 69160.366 10.356 0.768 1.00 0.00 H 959 2HG2 THR A 69158.743 10.129 0.117 1.00 0.00 H ATOM 960 3HG2 THR A 69159.982 10.920 -0.858 1.00 0.00 H ATOM 961 N ARG A 70160.593 7.377 2.629 1.00 0.00 N **ATOM** 962 CA ARG A 70159.811 6.918 3.771 1.00 0.00 C **ATOM** 963 C ARGA 70158.618 7.835 4.018 1.00 0.00 C **ATOM** 964 O ARG A 70158.749 9.059 4.005 1.00 0.00 O **ATOM** 965 CB ARG A 70160.689 6.855 5.023 1.00 0.00 C **ATOM** 966 CG ARG A 70159.948 6.370 6.260 1.00 0.00 C **ATOM** ATOM 967 CD ARG A 70160.069 7.358 7.410 1.00 0.00 C 968 NE ARG A 70160.228 6.685 8.697 1.00 0.00 N **ATOM** 969 CZ ARG A 70161.380 6.178 9.131 1.00 0.00 C **ATOM** 970 NH1 ARG A 70162.475 6.264 8.385 1.00 0.00 N **ATOM** 971 NH2 ARG A 70161.437 5.582 10.315 1.00 0.00 N **ATOM** 972 H ARG A 70161.529 7.635 2.762 1.00 0.00 H **ATOM** 973 HA ARG A 70159.448 5.926 3.546 1.00 0.00 H ATOM 974 1HB ARG A 70161.513 6.181 4.838 1.00 0.00 H **ATOM** 975 2HB ARG A 70161.079 7.841 5.225 1.00 0.00 H **ATOM** 976 1HG ARG A 70158.904 6.245 6.016 1.00 0.00 H ATOM 977 2HG ARG A 70160.363 5.421 6.567 1.00 0.00 H **ATOM ATOM** 978 1HD ARG A 70160.928 7.989 7.237 1.00 0.00 H 979 2HD ARG A 70159.177 7.966 7.440 1.00 0.00 H ATOM 980 HE ARG A 70159.436 6.606 9.267 1.00 0.00 H **ATOM** 981 1HH1 ARG A 70162.438 6.711 7.492 1.00 0.00 H ATOM 982 2HH1 ARG A 70163.337 5.881 8.717 1.00 0.00 H **ATOM** 983 1HH2 ARG A 70160.615 5.515 10.880 1.00 0.00 H **ATOM** 984 2HH2 ARG A 70162.303 5.202 10.641 1.00 0.00 H **ATOM** 985 N TYR A 71157.454 7.233 4.243 1.00 0.00 N ATOM

986 CA TYR A 71156.236 7.995 4.494 1.00 0.00 C ATOM 987 C TYR A 71155.691 7.705 5.889 1.00 0.00 C ATOM 988 O TYR A 71155.213 8.606 6.578 1.00 0.00 O **ATOM ATOM** 989 CB TYR A 71155.177 7.661 3.442 1.00 0.00 C 990 CG TYR A 71155.365 8.402 2.137 1.00 0.00 C **ATOM** 991 CD1 TYR A 71155.369 7.722 0.925 1.00 0.00 C ATOM 992 CD2 TYR A 71155.540 9.780 2.117 1.00 0.00 C ATOM 993 CE1 TYR A 71155.542 8.396 -0.270 1.00 0.00 C ATOM 994 CE2 TYR A 71155.713 10.460 0.926 1.00 0.00 C ATOM 995 CZ TYR A 71155.713 9.764 -0.263 1.00 0.00 C **ATOM** 996 OH TYR A 71155.885 10.437 -1.451 1.00 0.00 O ATOM 997 H TYR A 71157.415 6.255 4.240 1.00 0.00 H ATOM 998 HA TYR A 71156.481 9.044 4.426 1.00 0.00 H ATOM 999 1HB TYR A 71155.209 6.604 3.230 1.00 0.00 H ATOM ATOM 1000 2HB TYR A 71154.202 7.916 3.831 1.00 0.00 H ATOM 1001 HD1 TYR A 71155.235 6.651 0.924 1.00 0.00 H ATOM 1002 HD2 TYR A 71155.541 10.323 3.050 1.00 0.00 H ATOM 1003 HE1 TYR A 71155.541 7.849 -1.202 1.00 0.00 H ATOM 1004 HE2 TYR A 71155.847 11.532 0.931 1.00 0.00 H ATOM 1005 HH TYR A 71155.181 10.199 -2.060 1.00 0.00 H ATOM 1006 N PHE A 72155.770 6.445 6.299 1.00 0.00 N ATOM 1007 CA PHE A 72155.285 6.036 7.613 1.00 0.00 C ATOM 1008 C PHE A 72156.210 4.994 8.234 1.00 0.00 C ATOM 1009 O PHE A 72157.229 4.626 7.649 1.00 0.00 O ATOM 1010 CB PHE A 72153.866 5.476 7.505 1.00 0.00 C ATOM 1011 CG PHE A 72153.694 4.488 6.386 1.00 0.00 C ATOM 1012 CD1 PHE A 72153.520 4.923 5.082 1.00 0.00 C ATOM 1013 CD2 PHE A 72153.705 3.126 6.639 1.00 0.00 C ATOM 1014 CE1 PHE A 72153.360 4.017 4.050 1.00 0.00 C ATOM 1015 CE2 PHE A 72153.546 2.215 5.612 1.00 0.00 C ATOM 1016 CZ PHE A 72153.374 2.662 4.316 1.00 0.00 C

ATOM 1017 H PHE A 72156.163 5.772 5.705 1.00 0.00 H ATOM 1018 HA PHE A 72155,270 6,910 8,247 1,00 0,00 H ATOM 1019 1HB PHE A 72153.612 4.977 8.429 1.00 0.00 H ATOM 1020 2HB PHE A 72153.176 6.290 7.341 1.00 0.00 H ATOM 1021 HD1 PHE A 72153.509 5.983 4.874 1.00 0.00 H ATOM 1022 HD2 PHE A 72153.839 2.776 7.652 1.00 0.00 H ATOM 1023 HE1 PHE A 72153.225 4.369 3.039 1.00 0.00 H ATOM 1024 HE2 PHE A 72153.557 1.156 5.822 1.00 0.00 H ATOM 1025 HZ PHE A 72153,250 1,952 3,511 1,00 0,00 H ATOM 1026 N THR A 73155.849 4.521 9.422 1.00 0.00 N ATOM 1027 CA THR A 73156.646 3.521 10.122 1.00 0.00 C ATOM 1028 C THR A 73155.862 2.224 10.297 1.00 0.00 C ATOM 1029 O THR A 73154.872 2.180 11.028 1.00 0.00 O ATOM 1030 CB THR A 73157.085 4.053 11.487 1.00 0.00 C ATOM 1031 OG1 THR A 73157.756 3.047 12.225 1.00 0.00 O ATOM 1032 CG2 THR A 73155.934 4.552 12.333 1.00 0.00 C ATOM 1033 H THR A 73155.026 4.853 9.839 1.00 0.00 H ATOM 1034 HA THR A 73157.523 3.320 9.526 1.00 0.00 H ATOM 1035 HB THR A 73157.767 4.877 11.339 1.00 0.00 H ATOM 1036 HG1 THR A 73158.668 3.311 12.370 1.00 0.00 H ATOM 1037 1HG2 THR A 73156.046 5.613 12.504 1.00 0.00 H ATOM 1038 2HG2 THR A 73155.932 4.033 13.281 1.00 0.00 H ATOM 1039 3HG2 THR A 73155.002 4.368 11.819 1.00 0.00 H ATOM 1040 N CYS A 74156.311 1.172 9.622 1.00 0.00 N ATOM 1041 CA CYS A 74155.651 -0.126 9.704 1.00 0.00 C ATOM 1042 C CYS A 74156.672 -1.259 9.654 1.00 0.00 C ATOM 1043 O CYS A 74157.867 -1.025 9.475 1.00 0.00 O ATOM 1044 CB CYS A 74154.644 -0.282 8.562 1.00 0.00 C ATOM 1045 SG CYS A 74152.993 0.348 8.944 1.00 0.00 S ATOM 1046 H CYS A 74157.105 1.270 9.056 1.00 0.00 H ATOM 1047 HA CYS A 74155.125 -0.172 10.644 1.00 0.00 H

ATOM 1048 1HB CYS A 74155.007 0.252 7.697 1.00 0.00 H ATOM 1049 2HB CYS A 74154.548 -1.330 8.318 1.00 0.00 H ATOM 1050 HG CYS A 74153.037 0.799 9.791 1.00 0.00 H ATOM 1051 N ALA A 75156.192 -2.488 9.816 1.00 0.00 N ATOM 1052 CA ALA A 75157.063 -3.657 9.791 1.00 0.00 C ATOM 1053 C ALAA 75157.708 -3.832 8.420 1.00 0.00 C ATOM 1054 O ALA A 75157.169 -3.385 7.408 1.00 0.00 O ATOM 1055 CB ALA A 75156.281 -4.906 10.171 1.00 0.00 C ATOM 1056 H ALA A 75155.231 -2.611 9.956 1.00 0.00 H ATOM 1057 HA ALA A 75157.840 -3.510 10.527 1.00 0.00 H ATOM 1058 1HB ALA A 75155.259 -4.806 9.836 1.00 0.00 H ATOM 1059 2HB ALA A 75156.298 -5.028 11.244 1.00 0.00 H ATOM 1060 3HB ALA A 75156.730 -5.769 9.703 1.00 0.00 H ATOM 1061 N LEU A 76158.864 -4.486 8.395 1.00 0.00 N ATOM 1062 CA LEU A 76159.583 -4.720 7.148 1.00 0.00 C ATOM 1063 C LEUA 76158.884 -5.784 6.309 1.00 0.00 C ATOM 1064 O LEUA 76158.277 -6.711 6.844 1.00 0.00 O ATOM 1065 CB LEU A 76161.023 -5.147 7.437 1.00 0.00 C ATOM 1066 CG LEU A 76161.915 -4.055 8.031 1.00 0.00 C ATOM 1067 CD1 LEU A 76161.985 -4.187 9.545 1.00 0.00 C ATOM 1068 CD2 LEU A 76163.309 -4.116 7.425 1.00 0.00 C ATOM 1069 H LEU A 76159.244 -4.819 9.235 1.00 0.00 H ATOM 1070 HA LEU A 76159.597 -3.794 6.595 1.00 0.00 H ATOM 1071 1HB LEU A 76160.998 -5.979 8.127 1.00 0.00 H ATOM 1072 2HB LEU A 76161.469 -5.483 6.513 1.00 0.00 H ATOM 1073 HG LEU A 76161.491 -3.088 7.800 1.00 0.00 H ATOM 1074 1HD1 LEU A 76161.129 -4.740 9.897 1.00 0.00 H ATOM 1075 2HD1 LEU A 76161.987 -3.203 9.991 1.00 0.00 H ATOM 1076 3HD1 LEU A 76162.890 -4.708 9.819 1.00 0.00 H ATOM 1077 1HD2 LEU A 76163.238 -4.403 6.386 1.00 0.00 H ATOM 1078 2HD2 LEU A 76163.903 -4.844 7.959 1.00 0.00 H ATOM 1079 3HD2 LEU A 76163.778 -3.146 7.499 1.00 0.00 H ATOM 1080 N LYS A 77158.974 -5.644 4.990 1.00 0.00 N ATOM 1081 CA LYS A 77158.350 -6.593 4.075 1.00 0.00 C ATOM 1082 C LYS A 77156.836 -6.610 4.257 1.00 0.00 C ATOM 1083 O LYS A 77156.193 -7.648 4.097 1.00 0.00 O ATOM 1084 CB LYS A 77158.918 -7.997 4.297 1.00 0.00 C ATOM 1085 CG LYS A 77160.436 -8.038 4.345 1.00 0.00 C ATOM 1086 CD LYS A 77161.044 -7.809 2.971 1.00 0.00 C ATOM 1087 CE LYS A 77162.497 -7.372 3.069 1.00 0.00 C ATOM 1088 NZ LYS A 77163.335 -7.988 2.004 1.00 0.00 N ATOM 1089 H LYS A 77159.473 -4.884 4.623 1.00 0.00 H ATOM 1090 HA LYS A 77158.575 -6.278 3.067 1.00 0.00 H ATOM 1091 1HB LYS A 77158.538 -8.382 5.231 1.00 0.00 H ATOM 1092 2HB LYS A 77158.587 -8.637 3.492 1.00 0.00 H ATOM 1093 1HG LYS A 77160.787 -7.268 5.015 1.00 0.00 H ATOM 1094 2HG LYS A 77160.749 -9.005 4.710 1.00 0.00 H ATOM 1095 1HD LYS A 77160.993 -8.729 2.407 1.00 0.00 H ATOM 1096 2HD LYS A 77160.480 -7.041 2.462 1.00 0.00 H ATOM 1097 1HE LYS A 77162.544 -6.298 2.975 1.00 0.00 H ATOM 1098 2HE LYS A 77162.883 -7.667 4.034 1.00 0.00 H ATOM 1099 1HZ LYS A 77164.058 -7.312 1.683 1.00 0.00 H ATOM 1100 2HZ LYS A 77162.743 -8.255 1.192 1.00 0.00 H ATOM 1101 3HZ LYS A 77163.809 -8.840 2.368 1.00 0.00 H ATOM 1102 N LYS A 78156.273 -5.453 4.593 1.00 0.00 N ATOM 1103 CA LYS A 78154.833 -5.336 4.796 1.00 0.00 C ATOM 1104 C LYS A 78154.337 -3.953 4.387 1.00 0.00 C ATOM 1105 O LYS A 78153.462 -3.379 5.035 1.00 0.00 O ATOM 1106 CB LYS A 78154.482 -5.606 6.260 1.00 0.00 C ATOM 1107 CG LYS A 78154.975 -6.951 6.768 1.00 0.00 C ATOM 1108 CD LYS A 78154.548 -7.196 8.206 1.00 0.00 C ATOM 1109 CE LYS A 78153.329 -8.101 8.279 1.00 0.00 C

ATOM 1110 NZ LYS A 78152.528 -7.854 9.510 1.00 0.00 N ATOM 1111 H LYS A 78156.838 -4.661 4.705 1.00 0.00 H ATOM 1112 HA LYS A 78154.350 -6.076 4.177 1.00 0.00 H ATOM 1113 1HB LYS A 78154.920 -4.831 6.873 1.00 0.00 H ATOM 1114 2HB LYS A 78153.408 -5.575 6.372 1.00 0.00 H ATOM 1115 1HG LYS A 78154.567 -7.732 6.143 1.00 0.00 H ATOM 1116 2HG LYS A 78156.054 -6.971 6.712 1.00 0.00 H ATOM 1117 1HD LYS A 78155.363 -7.662 8.738 1.00 0.00 H ATOM 1118 2HD LYS A 78154.310 -6.247 8.667 1.00 0.00 H ATOM 1119 1HE LYS A 78152.709 -7.919 7.414 1.00 0.00 H ATOM 1120 2HE LYS A 78153.660 -9.129 8.274 1.00 0.00 H ATOM 1121 1HZ LYS A 78151.535 -8.120 9.347 1.00 0.00 H ATOM 1122 2HZ LYS A 78152.568 -6.849 9.768 1.00 0.00 H ATOM 1123 3HZ LYS A 78152.903 -8.419 10.299 1.00 0.00 H ATOM 1124 N ALA A 79154.903 -3.423 3.306 1.00 0.00 N ATOM 1125 CA ALAA 79154.517 -2.107 2.811 1.00 0.00 C ATOM 1126 C ALA A 79154.453 -2.093 1.287 1.00 0.00 C ATOM 1127 O ALAA 79155.479 -1.991 0.614 1.00 0.00 O ATOM 1128 CB ALAA 79155.491 -1.050 3.310 1.00 0.00 C ATOM 1129 H ALA A 79155.595 -3.929 2.832 1.00 0.00 H ATOM 1130 HA ALAA 79153.538 -1.876 3.204 1.00 0.00 H ATOM 1131 1HB ALAA 79154.952 -0.139 3.526 1.00 0.00 H ATOM 1132 2HB ALA A 79156.234 -0.858 2.551 1.00 0.00 H ATOM 1133 3HB ALA A 79155.976 -1.402 4.208 1.00 0.00 H ATOM 1134 N LEU A 80153.242 -2.196 0.749 1.00 0.00 N ATOM 1135 CA LEU A 80153.045 -2.195 -0.696 1.00 0.00 C ATOM 1136 C LEU A 80152.259 -0.964 -1.137 1.00 0.00 C ATOM 1137 O LEUA 80151.060 -0.857 -0.880 1.00 0.00 O ATOM 1138 CB LEU A 80152.312 -3.465 -1.132 1.00 0.00 C ATOM 1139 CG LEUA 80152.003 -3.553 -2.627 1.00 0.00 C ATOM 1140 CD1 LEU A 80153.212 -4.072 -3.391 1.00 0.00 C ATOM 1141 CD2 LEU A 80150.795 -4.445 -2.870 1.00 0.00 C ATOM 1142 H LEU A 80152.462 -2.275 1.338 1.00 0.00 H ATOM 1143 HA LEU A 80154.018 -2.173 -1.164 1.00 0.00 H ATOM 1144 1HB LEU A 80152.919 -4.317 -0.859 1.00 0.00 H ATOM 1145 2HB LEU A 80151.379 -3.521 -0.592 1.00 0.00 H ATOM 1146 HG LEUA 80151.773 -2.566 -3.000 1.00 0.00 H ATOM 1147 1HD1 LEU A 80154.113 -3.837 -2.843 1.00 0.00 H ATOM 1148 2HD1 LEU A 80153.251 -3.604 -4.364 1.00 0.00 H ATOM 1149 3HD1 LEU A 80153.131 -5.142 -3.509 1.00 0.00 H ATOM 1150 1HD2 LEU A 80149.892 -3.857 -2.792 1.00 0.00 H ATOM 1151 2HD2 LEU A 80150.775 -5.234 -2.131 1.00 0.00 H ATOM 1152 3HD2 LEU A 80150.858 -4.877 -3.857 1.00 0.00 H ATOM 1153 N PHE A 81152.943 -0.039 -1.802 1.00 0.00 N ATOM 1154 CA PHE A 81152.309 1.184 -2.279 1.00 0.00 C ATOM 1155 C PHE A 81151.493 0.917 -3.540 1.00 0.00 C ATOM 1156 O PHE A 81151.877 0.102 -4.379 1.00 0.00 O ATOM 1157 CB PHE A 81153.364 2.255 -2.559 1.00 0.00 C ATOM 1158 CG PHE A 81154.090 2.718 -1.328 1.00 0.00 C ATOM 1159 CD1 PHE A 81155.218 2.048 -0.880 1.00 0.00 C ATOM 1160 CD2 PHE A 81153.645 3.822 -0.619 1.00 0.00 C ATOM 1161 CE1 PHE A 81155.888 2.471 0.252 1.00 0.00 C ATOM 1162 CE2 PHE A 81154.311 4.250 0.515 1.00 0.00 C ATOM 1163 CZ PHE A 81155.435 3.573 0.950 1.00 0.00 C ATOM 1164 H PHE A 81153.896 -0.182 -1.977 1.00 0.00 H ATOM 1165 HA PHE A 81151.646 1.538 -1.505 1.00 0.00 H ATOM 1166 1HB PHE A 81154.096 1.859 -3.247 1.00 0.00 H ATOM 1167 2HB PHE A 81152.885 3.115 -3.006 1.00 0.00 H ATOM 1168 HD1 PHE A 81155.574 1.187 -1.426 1.00 0.00 H ATOM 1169 HD2 PHE A 81152.767 4.351 -0.958 1.00 0.00 H ATOM 1170 HE1 PHE A 81156.766 1.940 0.591 1.00 0.00 H ATOM 1171 HE2 PHE A 81153.954 5.111 1.059 1.00 0.00 H

ATOM 1172 HZ PHE A 81155.957 3.906 1.835 1.00 0.00 H ATOM 1173 N VALA 82150.364 1.608 -3.667 1.00 0.00 N ATOM 1174 CA VAL A 82149.494 1.444 -4.825 1.00 0.00 C ATOM 1175 C VALA 82148.612 2.671 -5.027 1.00 0.00 C ATOM 1176 O VALA 82148.497 3.519 -4.142 1.00 0.00 O ATOM 1177 CB VAL A 82148.598 0.200 -4.684 1.00 0.00 C ATOM 1178 CG1 VAL A 82149.428 -1.071 -4.779 1.00 0.00 C ATOM 1179 CG2 VAL A 82147.827 0.243 -3.373 1.00 0.00 C ATOM 1180 H VALA 82150.111 2.242 -2.965 1.00 0.00 H ATOM 1181 HA VALA 82150.120 1.314 -5.697 1.00 0.00 H ATOM 1182 HB VALA 82147.885 0.200 -5.496 1.00 0.00 H ATOM 1183 1HG1 VAL A 82150.036 -1.038 -5.671 1.00 0.00 H ATOM 1184 2HG1 VAL A 82148.771 -1.927 -4.824 1.00 0.00 H ATOM 1185 3HG1 VALA 82150.066 -1.150 -3.912 1.00 0.00 H ATOM 1186 1HG2 VAL A 82148.388 0.808 -2.643 1.00 0.00 H ATOM 1187 2HG2 VAL A 82147.675 -0.762 -3.011 1.00 0.00 H ATOM 1188 3HG2 VAL A 82146.869 0.716 -3.534 1.00 0.00 H ATOM 1189 N LYS A 83147.991 2.760 -6.199 1.00 0.00 N ATOM 1190 CA LYS A 83147.118 3.884 -6.518 1.00 0.00 C ATOM 1191 C LYS A 83145.833 3.826 -5.700 1.00 0.00 C ATOM 1192 O LYS A 83145.108 2.831 -5.732 1.00 0.00 O ATOM 1193 CB LYS A 83146.786 3.890 -8.012 1.00 0.00 C ATOM 1194 CG LYS A 83148.004 4.058 -8.904 1.00 0.00 C ATOM 1195 CD LYS A 83147.623 4.036 -10.376 1.00 0.00 C ATOM 1196 CE LYS A 83148.408 5.068-11.171 1.00 0.00 C ATOM 1197 NZ LYS A 83148.692 4.605 -12.557 1.00 0.00 N ATOM 1198 H LYS A 83148.122 2.052 -6.864 1.00 0.00 H ATOM 1199 HA LYS A 83147.645 4.793 -6.272 1.00 0.00 H ATOM 1200 1HB LYS A 83146.305 2.957 -8.265 1.00 0.00 H ATOM 1201 2HB LYS A 83146.104 4.703 -8.214 1.00 0.00 H ATOM 1202 1HG LYS A 83148.476 5.002 -8.680 1.00 0.00 H

ATOM 1203 2HG LYS A 83148.695 3.251 -8.709 1.00 0.00 H ATOM 1204 1HD LYS A 83147.829 3.055 -10.778 1.00 0.00 H ATOM 1205 2HD LYS A 83146.568 4.250 -10.469 1.00 0.00 H ATOM 1206 1HE LYS A 83147.833 5.980 -11.217 1.00 0.00 H ATOM 1207 2HE LYS A 83149.343 5.258 -10.664 1.00 0.00 H ATOM 1208 1HZ LYS A 83147.835 4.193 -12.979 1.00 0.00 H ATOM 1209 2HZ LYS A 83149.440 3.882 -12.546 1.00 0.00 H ATOM 1210 3HZ LYS A 83149.006 5.404 -13.143 1.00 0.00 H ATOM 1211 N LEUA 84145.559 4.900 -4.967 1.00 0.00 N ATOM 1212 CA LEU A 84144.362 4.977 -4.138 1.00 0.00 C ATOM 1213 C LEU A 84143.103 4.813 -4.985 1.00 0.00 C ATOM 1214 O LEU A 84142.124 4.210 -4.547 1.00 0.00 O ATOM 1215 CB LEU A 84144.324 6.314 -3.395 1.00 0.00 C ATOM 1216 CG LEU A 84143.055 6.569 -2.580 1.00 0.00 C ATOM 1217 CD1 LEU A 84143.085 5.777 -1.283 1.00 0.00 C ATOM 1218 CD2 LEU A 84142.896 8.055 -2.295 1.00 0.00 C ATOM 1219 H LEUA 84146.177 5.660 -4.986 1.00 0.00 H ATOM 1220 HA LEU A 84144.405 4.175 -3.419 1.00 0.00 H ATOM 1221 1HB LEU A 84145.170 6.352 -2.725 1.00 0.00 H ATOM 1222 2HB LEU A 84144.426 7.107 -4.120 1.00 0.00 H ATOM 1223 HG LEU A 84142.197 6.243 -3.150 1.00 0.00 H ATOM 1224 1HD1 LEU A 84142.799 4.753 -1.479 1.00 0.00 H ATOM 1225 2HD1 LEU A 84142.394 6.214 -0.577 1.00 0.00 H ATOM 1226 3HD1 LEU A 84144.083 5.798 -0.870 1.00 0.00 H ATOM 1227 1HD2 LEU A 84143.784 8.425 -1.805 1.00 0.00 H ATOM 1228 2HD2 LEU A 84142.040 8.209 -1.654 1.00 0.00 H ATOM 1229 3HD2 LEU A 84142.750 8.586 -3.224 1.00 0.00 H ATOM 1230 N LYS A 85143.138 5.352 -6.199 1.00 0.00 N ATOM 1231 CA LYS A 85141.999 5.264 -7.106 1.00 0.00 C ATOM 1232 C LYS A 85141.717 3.814 -7.488 1.00 0.00 C ATOM 1233 O LYS A 85140.589 3.461 -7.832 1.00 0.00 O

ATOM 1234 CB LYS A 85142.259 6.093 -8.365 1.00 0.00 C ATOM 1235 CG LYS A 85143.453 5.615 -9.173 1.00 0.00 C ATOM 1236 CD LYS A 85143.781 6.575 -10.306 1.00 0.00 C ATOM 1237 CE LYS A 85144.955 7.474 -9.953 1.00 0.00 C ATOM 1238 NZ LYS A 85144.679 8.301 -8.746 1.00 0.00 N ATOM 1239 H LYS A 85143.948 5.819 -6.491 1.00 0.00 H ATOM 1240 HA LYS A 85141.137 5.662 -6.595 1.00 0.00 H ATOM 1241 1HB LYS A 85141.384 6.050 -8.997 1.00 0.00 H ATOM 1242 2HB LYS A 85142.433 7.118 -8.077 1.00 0.00 H ATOM 1243 1HG LYS A 85144.310 5.538 -8.521 1.00 0.00 H ATOM 1244 2HG LYS A 85143.229 4.643 -9.590 1.00 0.00 H ATOM 1245 1HD LYS A 85144.031 6.004 -11.188 1.00 0.00 H ATOM 1246 2HD LYS A 85142.914 7.189 -10.506 1.00 0.00 H ATOM 1247 1HE LYS A 85145.821 6.858 -9.766 1.00 0.00 H ATOM 1248 2HE LYS A 85145.154 8.129 -10.789 1.00 0.00 H ATOM 1249 1HZ LYS A 85145.546 8.784 -8.437 1.00 0.00 H ATOM 1250 2HZ LYS A 85144.337 7.698 -7.970 1.00 0.00 H ATOM 1251 3HZ LYS A 85143.953 9.015 -8.959 1.00 0.00 H ATOM 1252 N SER A 86142.750 2.976 -7.427 1.00 0.00 N ATOM 1253 CA SER A 86142.608 1.565 -7.767 1.00 0.00 C ATOM 1254 C SER A 86142.494 0.710 -6.509 1.00 0.00 C ATOM 1255 O SER A 86142.923 -0.444 -6.490 1.00 0.00 O ATOM 1256 CB SER A 86143.800 1.100 -8.607 1.00 0.00 C ATOM 1257 OG SER A 86143.657 1.500 -9.959 1.00 0.00 O ATOM 1258 H SER A 86143.625 3.314 -7.147 1.00 0.00 H ATOM 1259 HA SER A 86141.704 1.453 -8.347 1.00 0.00 H ATOM 1260 1HB SER A 86144.707 1.531 -8.211 1.00 0.00 H ATOM 1261 2HB SER A 86143.866 0.023 -8.568 1.00 0.00 H ATOM 1262 HG SER A 86143.468 2.440 -9.997 1.00 0.00 H ATOM 1263 N CYS A 87141.913 1.284 -5.460 1.00 0.00 N ATOM 1264 CA CYS A 87141.742 0.575 -4.198 1.00 0.00 C

ATOM 1265 C CYS A 87140.267 0.304 -3.923 1.00 0.00 C ATOM 1266 O CYS A 87139.397 1.064 -4.346 1.00 0.00 O ATOM 1267 CB CYS A 87142.347 1.382 -3.048 1.00 0.00 C ATOM 1268 SG CYS A 87144.153 1.474 -3.081 1.00 0.00 S ATOM 1269 H CYS A 87141.592 2.207 -5.537 1.00 0.00 H ATOM 1270 HA CYS A 87142.262 -0.369 -4.274 1.00 0.00 H ATOM 1271 1HB CYS A 87141.968 2.393 -3.089 1.00 0.00 H ATOM 1272 2HB CYS A 87142.057 0.933 -2.110 1.00 0.00 H ATOM 1273 HG CYS A 87144.471 1.371 -2.181 1.00 0.00 H ATOM 1274 N ARG A 88139.992 -0.786 -3.212 1.00 0.00 N ATOM 1275 CA ARG A 88138.620 -1.156 -2.882 1.00 0.00 C ATOM 1276 C ARG A 88138.440 -1.289 -1.372 1.00 0.00 C ATOM 1277 O ARG A 88139.327 -1.781 -0.674 1.00 0.00 O ATOM 1278 CB ARG A 88138.247 -2.472 -3.569 1.00 0.00 C ATOM 1279 CG ARG A 88137.641 -2.286 -4.950 1.00 0.00 C ATOM 1280 CD ARG A 88136.123 -2.374 -4.909 1.00 0.00 C ATOM 1281 NE ARGA 88135.530 -2.222 -6.236 1.00 0.00 N ATOM 1282 CZ ARG A 88135.476 -1.068 -6.897 1.00 0.00 C ATOM 1283 NH1 ARG A 88135.977 0.037 -6.359 1.00 0.00 N ATOM 1284 NH2 ARG A 88134.919 -1.019 -8.099 1.00 0.00 N ATOM 1285 H ARG A 88140.729 -1.354 -2.903 1.00 0.00 H ATOM 1286 HA ARG A 88137.971 -0.374 -3.246 1.00 0.00 H ATOM 1287 1HB ARG A 88139.136 -3.077 -3.669 1.00 0.00 H ATOM 1288 2HB ARG A 88137.533 -2.997 -2.953 1.00 0.00 H ATOM 1289 1HG ARG A 88137.924 -1.316 -5.330 1.00 0.00 H ATOM 1290 2HG ARG A 88138.019 -3.056 -5.606 1.00 0.00 H ATOM 1291 1HD ARG A 88135.842 -3.335 -4.507 1.00 0.00 H ATOM 1292 2HD ARG A 88135.749 -1.591 -4.265 1.00 0.00 H ATOM 1293 HE ARG A 88135.152 -3.023 -6.656 1.00 0.00 H ATOM 1294 1HH1 ARG A 88136.399 0.007 -5.453 1.00 0.00 H ATOM 1295 2HH1 ARG A 88135.934 0.901 -6.861 1.00 0.00 H ATOM 1296 1HH2 ARG A 88134.539 -1.848 -8.509 1.00 0.00 H ATOM 1297 2HH2 ARG A 88134.878 -0.152 -8.596 1.00 0.00 H ATOM 1298 N PRO A 89137.282 -0.854 -0.841 1.00 0.00 N ATOM 1299 CA PRO A 89136.995 -0.931 0.595 1.00 0.00 C ATOM 1300 C PRO A 89137.153 -2.347 1.140 1.00 0.00 C ATOM 1301 O PRO A 89136.565 -3.293 0.616 1.00 0.00 O ATOM 1302 CB PRO A 89135.534 -0.482 0.696 1.00 0.00 C ATOM 1303 CG PRO A 89135.303 0.344 -0.521 1.00 0.00 C ATOM 1304 CD PRO A 89136.166 -0.254 -1.596 1.00 0.00 C ATOM 1305 HA PRO A 89137.622 -0.257 1.160 1.00 0.00 H ATOM 1306 1HB PRO A 89134.889 -1.349 0.715 1.00 0.00 H ATOM 1307 2HB PRO A 89135.394 0.097 1.597 1.00 0.00 H ATOM 1308 1HG PRO A 89134.262 0.297 -0.805 1.00 0.00 H ATOM 1309 2HG PRO A 89135.596 1.367 -0.332 1.00 0.00 H ATOM 1310 1HD PRO A 89135.619 -1.009 -2.142 1.00 0.00 H ATOM 1311 2HD PRO A 89136.522 0.515 -2.265 1.00 0.00 H ATOM 1312 N ASPA 90137.949 -2.484 2.196 1.00 0.00 N ATOM 1313 CA ASP A 90138.183 -3.784 2.811 1.00 0.00 C ATOM 1314 C ASPA 90137.359 -3.937 4.086 1.00 0.00 C ATOM 1315 O ASPA 90137.749 -3.455 5.149 1.00 0.00 O ATOM 1316 CB ASP A 90139.668 -3.964 3.127 1.00 0.00 C ATOM 1317 CG ASP A 90140.101 -5.416 3.066 1.00 0.00 C ATOM 1318 OD1 ASP A 90139.932 -6.041 1.997 1.00 0.00 O ATOM 1319 OD2 ASP A 90140.609 -5.928 4.085 1.00 0.00 O ATOM 1320 H ASPA 90138.389 -1.691 2.569 1.00 0.00 H ATOM 1321 HA ASP A 90137.878 -4.544 2.107 1.00 0.00 H ATOM 1322 1HB ASP A 90140.253 -3.403 2.413 1.00 0.00 H ATOM 1323 2HB ASP A 90139.866 -3.589 4.120 1.00 0.00 H ATOM 1324 N SER A 91136.220 -4.611 3.972 1.00 0.00 N ATOM 1325 CA SER A 91135.343 -4.826 5.118 1.00 0.00 C ATOM 1326 C SER A 91135.563 -6.209 5.723 1.00 0.00 C

ATOM 1327 O SER A 91134.646 -6.803 6.289 1.00 0.00 O ATOM 1328 CB SER A 91133.879 -4.667 4.702 1.00 0.00 C ATOM 1329 OG SER A 91133.091 -4.194 5.781 1.00 0.00 O ATOM 1330 H SER A 91135.962 -4.972 3.098 1.00 0.00 H ATOM 1331 HA SER A 91135.579 -4.079 5.859 1.00 0.00 H ATOM 1332 1HB SER A 91133.812 -3.962 3.887 1.00 0.00 H ATOM 1333 2HB SER A 91133.492 -5.624 4.383 1.00 0.00 H ATOM 1334 HG SER A 91132.300 -4.732 5.861 1.00 0.00 H ATOM 1335 N ARG A 92136.787 -6.715 5.600 1.00 0.00 N ATOM 1336 CA ARG A 92137.126 -8.028 6.137 1.00 0.00 C ATOM 1337 C ARG A 92137.058 -8.025 7.660 1.00 0.00 C ATOM 1338 O ARG A 92136.757 -9.045 8.281 1.00 0.00 O ATOM 1339 CB ARG A 92138.525 -8.444 5.677 1.00 0.00 C ATOM 1340 CG ARG A 92138.648 -8.601 4.171 1.00 0.00 C ATOM 1341 CD ARG A 92137.984 -9.879 3.686 1.00 0.00 C ATOM 1342 NE ARG A 92136.678 -9.622 3.082 1.00 0.00 N ATOM 1343 CZ ARG A 92136.048 -10.481 2.285 1.00 0.00 C ATOM 1344 NH1 ARG A 92136.599 -11.654 1.994 1.00 0.00 N ATOM 1345 NH2 ARG A 92134.864 -10.169 1.777 1.00 0.00 N ATOM 1346 H ARG A 92137.477 -6.195 5.139 1.00 0.00 H ATOM 1347 HA ARG A 92136.406 -8.738 5.757 1.00 0.00 H ATOM 1348 1HB ARG A 92139.234 -7.696 5.999 1.00 0.00 H ATOM 1349 2HB ARG A 92138.776 -9.388 6.138 1.00 0.00 H ATOM 1350 1HG ARG A 92138.176 -7.758 3.690 1.00 0.00 H ATOM 1351 2HG ARG A 92139.696 -8.627 3.906 1.00 0.00 H ATOM 1352 1HD ARG A 92138.623 -10.346 2.952 1.00 0.00 H ATOM 1353 2HD ARG A 92137.856 -10.545 4.527 1.00 0.00 H ATOM 1354 HE ARG A 92136.248 -8.764 3.281 1.00 0.00 H ATOM 1355 1HH1 ARG A 92137.492 -11.896 2.373 1.00 0.00 H ATOM 1356 2HH1 ARG A 92136.120 -12.295 1.395 1.00 0.00 H ATOM 1357 1HH2 ARG A 92134.444 -9.288 1.993 1.00 0.00 H

ATOM 1358 2HH2 ARG A 92134.390 -10.815 1.177 1.00 0.00 H ATOM 1359 N PHE A 93137.340 -6.872 8.258 1.00 0.00 N ATOM 1360 CA PHE A 93137.310 -6.734 9.709 1.00 0.00 C ATOM 1361 C PHE A 93136.350 -5.627 10.133 1.00 0.00 C ATOM 1362 O PHE A 93136.554 -4.973 11.155 1.00 0.00 O ATOM 1363 CB PHE A 93138.713 -6.439 10.243 1.00 0.00 C ATOM 1364 CG PHE A 93139.735 -7.465 9.842 1.00 0.00 C ATOM 1365 CD1 PHE A 93140.148 -7.570 8.523 1.00 0.00 C ATOM 1366 CD2 PHE A 93140.281 -8.323 10.782 1.00 0.00 C ATOM 1367 CE1 PHE A 93141.090 -8.512 8.151 1.00 0.00 C ATOM 1368 CE2 PHE A 93141.222 -9.267 10.416 1.00 0.00 C ATOM 1369 CZ PHE A 93141.626 -9.361 9.099 1.00 0.00 C ATOM 1370 H PHE A 93137.572 -6.093 7.709 1.00 0.00 H ATOM 1371 HA PHE A 93136.966 -7.671 10.124 1.00 0.00 H ATOM 1372 1HB PHE A 93139.039 -5.481 9.867 1.00 0.00 H ATOM 1373 2HB PHE A 93138.680 -6.406 11.321 1.00 0.00 H ATOM 1374 HD1 PHE A 93139.731 -6.905 7.782 1.00 0.00 H ATOM 1375 HD2 PHE A 93139.965 -8.250 11.813 1.00 0.00 H ATOM 1376 HE1 PHE A 93141.403 -8.585 7.120 1.00 0.00 H ATOM 1377 HE2 PHE A 93141.639 -9.930 11.159 1.00 0.00 H ATOM 1378 HZ PHE A 93142.361 -10.099 8.811 1.00 0.00 H ATOM 1379 N ALAA 94135.303 -5.421 9.339 1.00 0.00 N ATOM 1380 CA ALA A 94134.313 -4.393 9.632 1.00 0.00 C ATOM 1381 C ALAA 94133.083 -4.992 10.307 1.00 0.00 C ATOM 1382 O ALAA 94132.438 -5.889 9.763 1.00 0.00 O ATOM 1383 CB ALA A 94133.918 -3.663 8.357 1.00 0.00 C ATOM 1384 H ALA A 94135.195 -5.975 8.537 1.00 0.00 H ATOM 1385 HA ALAA 94134.765 -3.677 10.302 1.00 0.00 H ATOM 1386 1HB ALA A 94134.109 -2.606 8.472 1.00 0.00 H ATOM 1387 2HB ALA A 94132.867 -3.819 8.161 1.00 0.00 H ATOM 1388 3HB ALA A 94134.498 -4.044 7.530 1.00 0.00 H

ATOM 1389 N SER A 95132.763 -4.490 11.495 1.00 0.00 N ATOM 1390 CA SER A 95131.610 -4.975 12.245 1.00 0.00 C ATOM 1391 C SER A 95130.308 -4.529 11.587 1.00 0.00 C ATOM 1392 O SER A 95129.946 -3.354 11.637 1.00 0.00 O ATOM 1393 CB SER A 95131.664 -4.470 13.688 1.00 0.00 C ATOM 1394 OG SER A 95131.564 -3.058 13.739 1.00 0.00 O ATOM 1395 H SER A 95133.315 -3.776 11.877 1.00 0.00 H ATOM 1396 HA SER A 95131.648 -6.054 12.249 1.00 0.00 H ATOM 1397 1HB SER A 95130.845 -4.897 14.247 1.00 0.00 H ATOM 1398 2HB SER A 95132.600 -4.770 14.136 1.00 0.00 H ATOM 1399 HG SER A 95132.373 -2.667 13.400 1.00 0.00 H ATOM 1400 N LEU A 96129.608 -5.477 10.970 1.00 0.00 N ATOM 1401 CA LEU A 96128.346 -5.182 10.302 1.00 0.00 C ATOM 1402 C LEU A 96127.436 -6.404 10.293 1.00 0.00 C ATOM 1403 O LEUA 96126.247 -6.309 10.601 1.00 0.00 O ATOM 1404 CB LEU A 96128.601 -4.708 8.870 1.00 0.00 C ATOM 1405 CG LEU A 96127.648 -3.623 8.366 1.00 0.00 C ATOM 1406 CD1 LEU A 96128.191 -2.242 8.694 1.00 0.00 C ATOM 1407 CD2 LEU A 96127.421 -3.768 6.869 1.00 0.00 C ATOM 1408 H LEU A 96129.949 -6.395 10.965 1.00 0.00 H ATOM 1409 HA LEUA 96127.859 -4.393 10.851 1.00 0.00 H ATOM 1410 1HB LEU A 96129.611 -4.326 8.814 1.00 0.00 H ATOM 1411 2HB LEU A 96128.520 -5.561 8.212 1.00 0.00 H ATOM 1412 HG LEU A 96126.695 -3.733 8.862 1.00 0.00 H ATOM 1413 1HD1 LEU A 96129.269 -2.255 8.634 1.00 0.00 H ATOM 1414 2HD1 LEU A 96127.889 -1.963 9.694 1.00 0.00 H ATOM 1415 3HD1 LEU A 96127.801 -1.524 7.987 1.00 0.00 H ATOM 1416 1HD2 LEU A 96126.537 -4.363 6.695 1.00 0.00 H ATOM 1417 2HD2 LEU A 96128.275 -4.253 6.421 1.00 0.00 H ATOM 1418 3HD2 LEU A 96127.289 -2.790 6.429 1.00 0.00 H ATOM 1419 N GLN A 97128.003 -7.548 9.937 1.00 0.00 N

ATOM 1420 CA GLN A 97127.247 -8.794 9.885 1.00 0.00 C ATOM 1421 C GLN A 97126.955 -9.315 11.292 1.00 0.00 C ATOM 1422 O GLN A 97125.796 -9.457 11.681 1.00 0.00 O ATOM 1423 CB GLN A 97128.014 -9.848 9.081 1.00 0.00 C ATOM 1424 CG GLN A 97127.274 -10.326 7.843 1.00 0.00 C ATOM 1425 CD GLN A 97127.055 -9.219 6.831 1.00 0.00 C ATOM 1426 OE1 GLN A 97127.736 -8.193 6.859 1.00 0.00 O ATOM 1427 NE2 GLN A 97126.102 -9.421 5.929 1.00 0.00 N ATOM 1428 H GLN A 97128.953 -7.555 9.703 1.00 0.00 H ATOM 1429 HA GLN A 97126.309 -8.591 9.390 1.00 0.00 H ATOM 1430 1HB GLN A 97128.959 -9.428 8.770 1.00 0.00 H ATOM 1431 2HB GLN A 97128.202 -10.703 9.714 1.00 0.00 H ATOM 1432 1HG GLN A 97127.849 -11.112 7.376 1.00 0.00 H ATOM 1433 2HG GLN A 97126.311 -10.716 8.143 1.00 0.00 H ATOM 1434 1HE2 GLN A 97125.600 -10.262 5.967 1.00 0.00 H ATOM 1435 2HE2 GLN A 97125.939 -8.721 5.262 1.00 0.00 H ATOM 1436 N PRO A 98128.007 -9.608 12.075 1.00 0.00 N ATOM 1437 CA PRO A 98127.855 -10.116 13.442 1.00 0.00 C ATOM 1438 C PRO A 98127.388 -9.036 14.412 1.00 0.00 C ATOM 1439 O PRO A 98127.027 -7.933 14.001 1.00 0.00 O ATOM 1440 CB PRO A 98129.266 -10.584 13.802 1.00 0.00 C ATOM 1441 CG PRO A 98130.167 -9.736 12.973 1.00 0.00 C ATOM 1442 CD PRO A 98129.426 -9.470 11.691 1.00 0.00 C ATOM 1443 HA PRO A 98127.174 -10.952 13.480 1.00 0.00 H ATOM 1444 1HB PRO A 98129.439 -10.434 14.858 1.00 0.00 H ATOM 1445 2HB PRO A 98129.375 -11.630 13.558 1.00 0.00 H ATOM 1446 1HG PRO A 98130.372 -8.809 13.488 1.00 0.00 H ATOM 1447 2HG PRO A 98131.086 -10.266 12.772 1.00 0.00 H ATOM 1448 1HD PRO A 98129.634 -8.470 11.337 1.00 0.00 H ATOM 1449 2HD PRO A 98129.695 -10.199 10.941 1.00 0.00 H ATOM 1450 N SER A 99127.397 -9.361 15.700 1.00 0.00 N

ATOM 1451 CA SER A 99126.974 -8.420 16.730 1.00 0.00 C ATOM 1452 C SER A 99128.013 -8.325 17.842 1.00 0.00 C ATOM 1453 O SER A 99127.894 -8.984 18.875 1.00 0.00 O ATOM 1454 CB SER A 99125.624 -8.841 17.313 1.00 0.00 C ATOM 1455 OG SER A 99125.449 -10.245 17.232 1.00 0.00 O ATOM 1456 H SER A 99127.696 -10.257 15.965 1.00 0.00 H ATOM 1457 HA SER A 99126.869 -7.449 16.269 1.00 0.00 H ATOM 1458 1HB SER A 99125.573 -8.545 18.351 1.00 0.00 H ATOM 1459 2HB SER A 99124.830 -8.359 16.762 1.00 0.00 H ATOM 1460 HG SER A 99125.229 -10.489 16.329 1.00 0.00 H ATOM 1461 N GLY A 100129.034 -7.502 17.623 1.00 0.00 N ATOM 1462 CA GLY A 100130.080 -7.338 18.614 1.00 0.00 C ATOM 1463 C GLY A 100129.626 -6.514 19.806 1.00 0.00 C ATOM 1464 O GLY A 100128.689 -5.723 19.694 1.00 0.00 O ATOM 1465 H GLY A 100129.076 -7.003 16.780 1.00 0.00 H ATOM 1466 1HA GLY A 100130.389 -8.312 18.962 1.00 0.00 H ATOM 1467 2HA GLY A 100130.925 -6.847 18.153 1.00 0.00 H ATOM 1468 N PRO A 101130.277 -6.678 20.969 1.00 0.00 N ATOM 1469 CA PRO A 101129.924 -5.935 22.183 1.00 0.00 C ATOM 1470 C PRO A 101130.281 -4.456 22.081 1.00 0.00 C ATOM 1471 O PRO A 101130.835 -4.008 21.078 1.00 0.00 O ATOM 1472 CB PRO A 101130.760 -6.613 23.272 1.00 0.00 C ATOM 1473 CG PRO A 101131.923 -7.196 22.548 1.00 0.00 C ATOM 1474 CD PRO A 101131.408 -7.600 21.194 1.00 0.00 C ATOM 1475 HA PRO A 101128.874 -6.036 22.418 1.00 0.00 H ATOM 1476 1HB PRO A 101131.075 -5.877 23.998 1.00 0.00 H ATOM 1477 2HB PRO A 101130.173 -7.379 23.757 1.00 0.00 H ATOM 1478 1HG PRO A 101132.702 -6.456 22.446 1.00 0.00 H ATOM 1479 2HG PRO A 101132.292 -8.060 23.080 1.00 0.00 H ATOM 1480 1HD PRO A 101132.171 -7.462 20.442 1.00 0.00 H ATOM 1481 2HD PRO A 101131.071 -8.625 21.207 1.00 0.00 H ATOM 1482 N SER A 102129.959 -3.702 23.127 1.00 0.00 N ATOM 1483 CA SER A 102130.245 -2.272 23.156 1.00 0.00 C ATOM 1484 C SER A 102131.024 -1.897 24.413 1.00 0.00 C ATOM 1485 O SER A 102132.035 -1.200 24.344 1.00 0.00 O ATOM 1486 CB SER A 102128.945 -1.469 23.089 1.00 0.00 C ATOM 1487 OG SER A 102127.980 -2.124 22.284 1.00 0.00 O ATOM 1488 H SER A 102129.518 -4.116 23.899 1.00 0.00 H ATOM 1489 HA SER A 102130.847 -2.037 22.291 1.00 0.00 H ATOM 1490 1HB SER A 102128.544 -1.353 24.086 1.00 0.00 H ATOM 1491 2HB SER A 102129.146 -0.495 22.668 1.00 0.00 H ATOM 1492 HG SER A 102128.380 -2.382 21.450 1.00 0.00 H ATOM 1493 N SER A 103130.545 -2.367 25.561 1.00 0.00 N ATOM 1494 CA SER A 103131.197 -2.082 26.834 1.00 0.00 C ATOM 1495 C SER A 103130.874 -3.160 27.863 1.00 0.00 C ATOM 1496 O SER A 103131.771 -3.823 28.384 1.00 0.00 O ATOM 1497 CB SER A 103130,760 -0.712 27.358 1.00 0.00 C ATOM 1498 OG SER A 103131.620 0.311 26.891 1.00 0.00 O ATOM 1499 H SER A 103129.734 -2.918 25.551 1.00 0.00 H ATOM 1500 HA SER A 103132.262 -2.069 26.665 1.00 0.00 H ATOM 1501 1HB SER A 103129.756 -0.503 27.021 1.00 0.00 H ATOM 1502 2HB SER A 103130.783 -0.720 28.438 1.00 0.00 H ATOM 1503 HG SER A 103132.396 0.360 27.455 1.00 0.00 H ATOM 1504 N GLY A 104129.588 -3.329 28.153 1.00 0.00 N ATOM 1505 CA GLY A 104129.170 -4.328 29.119 1.00 0.00 C ATOM 1506 C GLY A 104127.832 -4.001 29.751 1.00 0.00 C ATOM 1507 O GLY A 104127.823 -3.345 30.815 1.00 0.00 O ATOM 1508 OXT GLY A 104126.794 -4.397 29.183 1.00 0.00 O ATOM 1509 H GLY A 104128.917 -2.771 27.707 1.00 0.00 H ATOM 1510 1HA GLY A 104129.097 -5.284 28.622 1.00 0.00 H ATOM 1511 2HA GLY A 104129.917 -4.395 29.897 1.00 0.00 H TER 1512 GLY A 104

ENDMDL

Three-Dimensional Structure Coordinate Table 8 ATOM 1 N GLY A 1135.862 21.326 -5.428 1.00 0.00 N ATOM 2 CA GLY A 1136.784 22.453 -5.740 1.00 0.00 C ATOM 3 C GLY A 1136.436 23.144 -7.044 1.00 0.00 C ATOM 4 O GLY A 1135.778 24.184 -7.046 1.00 0.00 O ATOM 5 1H GLY A 1134.965 21.447 -5.941 1.00 0.00 H ATOM 6 2H GLY A 1135.664 21.298 -4.408 1.00 0.00 H ATOM 7 3H GLY A 1136.294 20.423 -5.712 1.00 0.00 H ATOM 8 1HA GLY A 1136.736 23.175 -4.938 1.00 0.00 H ATOM 9 2HA GLY A 1137.793 22.071 -5.805 1.00 0.00 H ATOM10 N SER A 2136.880 22.565 -8.154 1.00 0.00 N ATOM11 CA SER A 2136.611 23.132 -9.471 1.00 0.00 C ATOM12 C SER A 2135.133 23.008 -9.825 1.00 0.00 C ATOM13 O SER A 2134.622 21.906 -10.024 1.00 0.00 O ATOM14 CB SER A 2137.463 22.432 -10.532 1.00 0.00 C ATOM15 OG SER A 2137.904 23.351 -11.518 1.00 0.00 O ATOM16 H SER A 2137.399 21.736 -8.087 1.00 0.00 H ATOM17 HA SER A 2136.876 24.178 -9.441 1.00 0.00 H ATOM18 1HB SER A 2138.326 21.986 -10.063 1.00 0.00 H ATOM19 2HB SER A 2136.876 21.663 -11.012 1.00 0.00 H ATOM20 HG SER A 2138.856 23.456 -11.454 1.00 0.00 H ATOM21 N SER A 3134.452 24.146 -9.904 1.00 0.00 N ATOM22 CA SER A 3133.032 24.166 -10.234 1.00 0.00 C ATOM23 C SER A 3132.822 24.039 -11.740 1.00 0.00 C ATOM24 O SER A 3133.076 24.979 -12.494 1.00 0.00 O ATOM25 CB SER A 3132.385 25.455 -9.725 1.00 0.00 C ATOM26 OG SER A 3132.929 26.590 -10.375 1.00 0.00 O ATOM27 H SER A 3134.915 24.993 -9.735 1.00 0.00 H ATOM28 HA SER A 3132.567 23.323 -9.747 1.00 0.00 H

ATOM29 1HB SER A 3131.323 25.422 -9.915 1.00 0.00 H ATOM30 2HB SER A 3132.558 25.547 -8.663 1.00 0.00 H ATOM31 HG SER A 3132.626 26.615 -11.286 1.00 0.00 H ATOM32 N GLY A 4132.358 22.871 -12.172 1.00 0.00 N ATOM33 CA GLY A 4132.122 22.643 -13.585 1.00 0.00 C ATOM34 C GLY A 4132.095 21.169 -13.938 1.00 0.00 C ATOM35 O GLY A 4132.285 20.314 -13.073 1.00 0.00 O ATOM36 H GLY A 4132.174 22.159 -11.525 1.00 0.00 H ATOM37 1HA GLY A 4131.175 23.084 -13.857 1.00 0.00 H ATOM38 2HA GLY A 4132.906 23.123 -14.151 1.00 0.00 H ATOM39 N SER A 5131.857 20.871 -15.211 1.00 0.00 N ATOM40 CA SER A 5131.806 19.490 -15.676 1.00 0.00 C ATOM41 C SER A 5130.700 18.717 -14.963 1.00 0.00 C ATOM42 O SER A 5130.136 19.190 -13.977 1.00 0.00 O ATOM43 CB SER A 5133.153 18.803 -15.448 1.00 0.00 C ATOM44 OG SER A 5133.460 17.916 -16.510 1.00 0.00 O ATOM45 H SER A 5131.714 21.598 -15.853 1.00 0.00 H ATOM46 HA SER A 5131.593 19.505 -16.734 1.00 0.00 H ATOM47 1HB SER A 5133.930 19.550 -15.385 1.00 0.00 H ATOM48 2HB SER A 5133.118 18.242 -14.526 1.00 0.00 H ATOM49 HG SER A 5133.809 18.414 -17.252 1.00 0.00 H ATOM50 N SER A 6130.397 17.527 -15.469 1.00 0.00 N ATOM51 CA SER A 6129.360 16.689 -14.880 1.00 0.00 C ATOM52 C SER A 6129.754 15.216 -14.934 1.00 0.00 C ATOM53 O SER A 6129.519 14.536 -15.934 1.00 0.00 O ATOM54 CB SER A 6128.031 16.900 -15.608 1.00 0.00 C ATOM55 OG SER A 6128.003 18.156 -16.264 1.00 0.00 O ATOM56 H SER A 6130.884 17.203 -16.256 1.00 0.00 H ATOM57 HA SER A 6129.244 16.980 -13.847 1.00 0.00 H ATOM58 1HB SER A 6127.897 16.121 -16.343 1.00 0.00 H ATOM59 2HB SER A 6127.222 16.863 -14.893 1.00 0.00 H ATOM60 HG SER A 6127.925 18.856 -15.612 1.00 0.00 H ATOM61 N GLY A 7130.352 14.729 -13.853 1.00 0.00 N ATOM62 CA GLY A 7130.769 13.340 -13.798 1.00 0.00 C ATOM63 C GLY A 7131.372 12.967 -12.458 1.00 0.00 C ATOM64 O GLY A 7132.589 12.825 -12.335 1.00 0.00 O ATOM65 H GLY A 7130.513 15.317 -13.085 1.00 0.00 H ATOM66 1HA GLY A 7129.910 12.711 -13.981 1.00 0.00 H ATOM67 2HA GLY A 7131.502 13.165 -14.571 1.00 0.00 H ATOM68 N LEUA 8130.520 12.809 -11.450 1.00 0.00 N ATOM69 CA LEU A 8130.974 12.451 -10.112 1.00 0.00 C ATOM70 C LEUA 8130.399 11.105 -9.684 1.00 0.00 C ATOM71 O LEUA 8129.312 10.718 -10.114 1.00 0.00 O ATOM72 CB LEU A 8130.573 13.532 -9.107 1.00 0.00 C ATOM73 CG LEU A 8130.735 14.970 -9.605 1.00 0.00 C ATOM74 CD1 LEU A 8129.892 15.921 -8.770 1.00 0.00 C ATOM75 CD2 LEU A 8132.199 15.382 -9.570 1.00 0.00 C ATOM76 H LEUA 8129.561 12.936 -11.611 1.00 0.00 H ATOM77 HA LEU A 8132.051 12.376 -10.136 1.00 0.00 H ATOM78 1HB LEU A 8129.538 13.379 -8.841 1.00 0.00 H ATOM79 2HB LEU A 8131.177 13.412 -8.221 1.00 0.00 H ATOM80 HG LEU A 8130.392 15.031 -10.627 1.00 0.00 H ATOM81 1HD1 LEU A 8129.871 16.892 -9.242 1.00 0.00 H ATOM82 2HD1 LEU A 8130.321 16.010 -7.782 1.00 0.00 H ATOM83 3HD1 LEU A 8128.885 15.537 -8.692 1.00 0.00 H ATOM84 1HD2 LEU A 8132.656 15.168 -10.525 1.00 0.00 H ATOM85 2HD2 LEU A 8132.710 14.832 -8.795 1.00 0.00 H ATOM86 3HD2 LEU A 8132.270 16.441 -9.367 1.00 0.00 H ATOM87 N ALAA 9131.134 10.395 -8.834 1.00 0.00 N ATOM88 CA ALA A 9130.696 9.092 -8.348 1.00 0.00 C ATOM89 C ALA A 9131.453 8.694 -7.086 1.00 0.00 C ATOM90 O ALAA 9131.772 7.522 -6.886 1.00 0.00 O

ATOM91 CB ALA A 9130.878 8.038 -9.430 1.00 0.00 C ATOM92 H ALAA 9131.991 10.756 -8.527 1.00 0.00 H ATOM93 HA ALA A 9129.643 9.160 -8.118 1.00 0.00 H ATOM94 1HB ALA A 9129.990 7.996 -10.045 1.00 0.00 H ATOM95 2HB ALA A 9131.042 7.075 -8.970 1.00 0.00 H ATOM96 3HB ALA A 9131.728 8.295 -10.044 1.00 0.00 H ATOM97 N MET A 10131.737 9.675 -6.238 1.00 0.00 N ATOM98 CA META 10132.457 9.427 -4.994 1.00 0.00 C ATOM99 C META 10132.314 10.608 -4.035 1.00 0.00 C 100 O META 10133.291 11.291 -3.728 1.00 0.00 O ATOM 101 CB META 10133.936 9.159 -5.280 1.00 0.00 C **ATOM** 102 CG META 10134.602 10.248 -6.106 1.00 0.00 C **ATOM** 103 SD META 10136.400 10.200 -5.997 1.00 0.00 S **ATOM** 104 CE META 10136.829 11.766 -6.751 1.00 0.00 C **ATOM** 105 H MET A 10131.456 10.589 -6.452 1.00 0.00 H **ATOM ATOM** 106 HA MET A 10132.025 8.550 -4.532 1.00 0.00 H **ATOM** 107 1HB MET A 10134.463 9.076 -4.342 1.00 0.00 H 108 2HB MET A 10134.023 8.226 -5.817 1.00 0.00 H ATOM 109 1HG META 10134.315 10.123 -7.140 1.00 0.00 H **ATOM** 110 2HG MET A 10134.259 11.209 -5.752 1.00 0.00 H ATOM **ATOM** 111 1HE META 10137.179 11.598 -7.758 1.00 0.00 H 112 2HE MET A 10137.606 12.244 -6.174 1.00 0.00 H **ATOM** 113 3HE MET A 10135.957 12.404 -6.776 1.00 0.00 H **ATOM** 114 N PRO A 11131.087 10.866 -3.550 1.00 0.00 N ATOM 115 CA PRO A 11130.821 11.971 -2.624 1.00 0.00 C **ATOM** 116 C PRO A 11131.642 11.867 -1.340 1.00 0.00 C ATOM 117 O PRO A 11132.251 12.845 -0.908 1.00 0.00 O ATOM 118 CB PRO A 11129.326 11.848 -2.315 1.00 0.00 C ATOM 119 CG PRO A 11128.762 11.010 -3.412 1.00 0.00 C ATOM 120 CD PRO A 11129.869 10.103 -3.867 1.00 0.00 C ATOM 121 HA PRO A 11131.015 12.926 -3.092 1.00 0.00 H ATOM

122 1HB PRO A 11129.192 11.379 -1.351 1.00 0.00 H **ATOM** 123 2HB PRO A 11128.878 12.831 -2.304 1.00 0.00 H **ATOM** 124 1HG PRO A 11127.936 10.427 -3.036 1.00 0.00 H ATOM 125 2HG PRO A 11128.436 11.641 -4.225 1.00 0.00 H **ATOM** 126 1HD PRO A 11129.843 9.171 -3.321 1.00 0.00 H **ATOM** 127 2HD PRO A 11129.794 9.920 -4.929 1.00 0.00 H **ATOM** 128 N PRO A 12131.677 10.677 -0.709 1.00 0.00 N ATOM 129 CA PRO A 12132.438 10.469 0.528 1.00 0.00 C **ATOM** 130 C PROA 12133.904 10.857 0.370 1.00 0.00 C **ATOM** 131 O PROA 12134.589 11.145 1.352 1.00 0.00 O **ATOM** 132 CB PRO A 12132.309 8.965 0.784 1.00 0.00 C **ATOM** 133 CG PRO A 12131.074 8.556 0.061 1.00 0.00 C ATOM 134 CD PRO A 12130.989 9.447 -1.146 1.00 0.00 C ATOM 135 HA PRO A 12132.008 11.017 1.353 1.00 0.00 H ATOM 136 1HB PRO A 12133.180 8.455 0.397 1.00 0.00 H **ATOM** 137 2HB PRO A 12132.223 8.783 1.845 1.00 0.00 H **ATOM** 138 1HG PRO A 12131.149 7.522 -0.240 1.00 0.00 H **ATOM** 139 2HG PRO A 12130.212 8.703 0.695 1.00 0.00 H **ATOM** 140 1HD PRO A 12131.501 8.996 -1.984 1.00 0.00 H **ATOM** 141 2HD PRO A 12129.959 9.647 -1.395 1.00 0.00 H **ATOM** 142 N GLY A 13134.378 10.862 -0.872 1.00 0.00 N **ATOM** 143 CA GLY A 13135.761 11.216 -1.136 1.00 0.00 C **ATOM** 144 C GLY A 13136.420 10.278 -2.127 1.00 0.00 C ATOM 145 O GLY A 13136.953 10.716 -3.146 1.00 0.00 O **ATOM** 146 H GLY A 13133.785 10.624 -1.616 1.00 0.00 H **ATOM** 147 1HA GLY A 13135.794 12.220 -1.531 1.00 0.00 H **ATOM** 148 2HA GLY A 13136.311 11.187 -0.208 1.00 0.00 H **ATOM** 149 N ASN A 14136.385 8.983 -1.827 1.00 0.00 N ATOM 150 CA ASN A 14136.984 7.980 -2.698 1.00 0.00 C ATOM 151 C ASN A 14136.171 6.690 -2.683 1.00 0.00 C ATOM 152 O ASN A 14136.322 5.861 -1.785 1.00 0.00 O ATOM

- ATOM 153 CB ASN A 14138.424 7.694 -2.268 1.00 0.00 C
- ATOM 154 CG ASN A 14139.315 8.916 -2.382 1.00 0.00 C
- ATOM 155 OD1 ASN A 14140.077 9.056 -3.338 1.00 0.00 O
- ATOM 156 ND2 ASN A 14139.222 9.809 -1.403 1.00 0.00 N
- ATOM 157 H ASN A 14135.946 8.697 -0.999 1.00 0.00 H
- ATOM 158 HA ASN A 14136.990 8.375 -3.704 1.00 0.00 H
- ATOM 159 1HB ASN A 14138.428 7.364 -1.240 1.00 0.00 H
- ATOM 160 2HB ASN A 14138.832 6.914 -2.894 1.00 0.00 H
- ATOM 161 1HD2 ASN A 14138.593 9.631 -0.673 1.00 0.00 H
- ATOM 162 2HD2 ASN A 14139.787 10.609 -1.451 1.00 0.00 H
- ATOM 163 N SER A 15135,310 6.527 -3.682 1.00 0.00 N
- ATOM 164 CA SER A 15134.470 5.338 -3.787 1.00 0.00 C
- ATOM 165 C SER A 15133.494 5.253 -2.616 1.00 0.00 C
- ATOM 166 O SER A 15132.317 5.585 -2.753 1.00 0.00 O
- ATOM 167 CB SER A 15135.336 4.076 -3.840 1.00 0.00 C
- ATOM 168 OG SER A 15135.576 3.678 -5.179 1.00 0.00 O
- ATOM 169 H SER A 15135.237 7.224 -4.368 1.00 0.00 H
- ATOM 170 HA SER A 15133.905 5.413 -4.704 1.00 0.00 H
- ATOM 171 1HB SER A 15136.284 4.272 -3.361 1.00 0.00 H
- ATOM 172 2HB SER A 15134.832 3.273 -3.323 1.00 0.00 H
- ATOM 173 HG SER A 15136.355 4.129 -5.512 1.00 0.00 H
- ATOM 174 N HIS A 16133.990 4.808 -1.466 1.00 0.00 N
- ATOM 175 CA HIS A 16133.161 4.680 -0.273 1.00 0.00 C
- ATOM 176 C HIS A 16133.758 5.463 0.892 1.00 0.00 C
- ATOM 177 O HIS A 16133.046 6.158 1.616 1.00 0.00 O
- ATOM 178 CB HIS A 16133.007 3.208 0.111 1.00 0.00 C
- ATOM 179 CG HIS A 16131.982 2.480 -0.703 1.00 0.00 C
- ATOM 180 ND1 HIS A 16130.635 2.772 -0.652 1.00 0.00 N
- ATOM 181 CD2 HIS A 16132.113 1.469 -1.593 1.00 0.00 C
- ATOM 182 CE1 HIS A 16129.982 1.969 -1.475 1.00 0.00 C
- ATOM 183 NE2 HIS A 16130.856 1.170 -2.059 1.00 0.00 N

184 H HIS A 16134.936 4.559 -1.419 1.00 0.00 H **ATOM** 185 HA HIS A 16132.187 5.087 -0.502 1.00 0.00 H ATOM 186 1HB HIS A 16133.953 2.708 -0.024 1.00 0.00 H ATOM 187 2HB HIS A 16132.715 3.143 1.149 1.00 0.00 H **ATOM** 188 HD1 HIS A 16130.219 3.462 -0.095 1.00 0.00 H ATOM 189 HD2 HIS A 16133.035 0.986 -1.884 1.00 0.00 H ATOM ATOM 190 HE1 HIS A 16128.915 1.969 -1.642 1.00 0.00 H 191 HE2 HIS A 16130.650 0.540 -2.779 1.00 0.00 H **ATOM** 192 N GLYA 17135.070 5.345 1.066 1.00 0.00 N **ATOM** 193 CA GLY A 17135.741 6.047 2.144 1.00 0.00 C **ATOM** 194 C GLYA 17137.087 5.436 2.485 1.00 0.00 C **ATOM ATOM** 195 O GLY A 17137.242 4.806 3.530 1.00 0.00 O 196 H GLYA 17135.587 4.777 0.457 1.00 0.00 H **ATOM** 197 1HA GLY A 17135.889 7.076 1.853 1.00 0.00 H **ATOM** 198 2HA GLY A 17135.113 6.019 3.022 1.00 0.00 H **ATOM** 199 N LEUA 18138.060 5.623 1.600 1.00 0.00 N ATOM 200 CA LEU A 18139.399 5.086 1.811 1.00 0.00 C ATOM 201 C LEU A 18140.344 6.167 2.328 1.00 0.00 C **ATOM** 202 O LEUA 18140.685 7.103 1.606 1.00 0.00 O ATOM 203 CB LEU A 18139.946 4.493 0.511 1.00 0.00 C **ATOM** 204 CG LEUA 18139.060 3.428 -0.138 1.00 0.00 C ATOM 205 CD1 LEU A 18139.482 3.188 -1.579 1.00 0.00 C **ATOM** 206 CD2 LEU A 18139.115 2.134 0.659 1.00 0.00 C ATOM 207 H LEUA 18137.874 6.134 0.784 1.00 0.00 H **ATOM** 208 HA LEUA 18139.328 4.303 2.551 1.00 0.00 H **ATOM** 209 1HB LEUA 18140.082 5.298 -0.196 1.00 0.00 H **ATOM** 210 2HB LEU A 18140.908 4.051 0.718 1.00 0.00 H **ATOM** 211 HG LEUA 18138.037 3.776 -0.144 1.00 0.00 H ATOM 212 1HD1 LEU A 18139.230 2.178 -1.864 1.00 0.00 H ATOM 213 2HD1 LEU A 18140.549 3.332 -1.670 1.00 0.00 H ATOM ATOM 214 3HD1 LEU A 18138.969 3.883 -2.226 1.00 0.00 H

215 1HD2 LEU A 18140.134 1.935 0.954 1.00 0.00 H 216 2HD2 LEU A 18138.751 1.320 0.050 1.00 0.00 H **ATOM** 217 3HD2 LEU A 18138.497 2.226 1.540 1.00 0.00 H ATOM **ATOM** 218 N GLUA 19140.763 6.029 3.581 1.00 0.00 N 219 CA GLUA 19141.670 6.993 4.194 1.00 0.00 C ATOM 220 C GLUA 19142.671 6.294 5.108 1.00 0.00 C **ATOM** 221 O GLUA 19142.581 5.089 5.338 1.00 0.00 O **ATOM** 222 CB GLUA 19140.878 8.036 4.986 1.00 0.00 C **ATOM ATOM** 223 CG GLU A 19139.943 7.432 6.022 1.00 0.00 C 224 CD GLUA 19138.972 8.446 6.592 1.00 0.00 C ATOM 225 OE1 GLU A 19138.749 8.429 7.820 1.00 0.00 O ATOM 226 OE2 GLU A 19138.435 9.259 5.810 1.00 0.00 O ATOM 227 H GLU A 19140.458 5.260 4.107 1.00 0.00 H ATOM ATOM 228 HA GLUA 19142.209 7.491 3.402 1.00 0.00 H 229 1HB GLU A 19141.573 8.686 5.497 1.00 0.00 H ATOM 230 2HB GLU A 19140.288 8.623 4.298 1.00 0.00 H ATOM 231 1HG GLU A 19139.378 6.637 5.558 1.00 0.00 H ATOM 232 2HG GLU A 19140.535 7.027 6.830 1.00 0.00 H ATOM ATOM 233 N VALA 20143.626 7.060 5.626 1.00 0.00 N **ATOM** 234 CA VALA 20144.644 6.514 6.516 1.00 0.00 C 235 C VALA 20144.014 5.893 7.757 1.00 0.00 C **ATOM** 236 O VALA 20143.157 6.499 8.401 1.00 0.00 O **ATOM** 237 CB VALA 20145.649 7.598 6.952 1.00 0.00 C **ATOM** 238 CG1 VAL A 20146.811 6.976 7.710 1.00 0.00 C ATOM ATOM 239 CG2 VAL A 20146.147 8.381 5.747 1.00 0.00 C 240 H VALA 20143.645 8.015 5.406 1.00 0.00 H ATOM 241 HA VALA 20145.184 5.750 5.976 1.00 0.00 H **ATOM** 242 HB VALA 20145.142 8.284 7.615 1.00 0.00 H ATOM 243 1HG1 VAL A 20147.087 6.042 7.244 1.00 0.00 H ATOM ATOM 244 2HG1 VAL A 20146.517 6.793 8.733 1.00 0.00 H ATOM 245 3HG1 VAL A 20147.655 7.650 7.693 1.00 0.00 H

246 1HG2 VAL A 20147.116 8.803 5.967 1.00 0.00 H ATOM 247 2HG2 VAL A 20145.451 9.175 5.521 1.00 0.00 H ATOM 248 3HG2 VAL A 20146.227 7.720 4.897 1.00 0.00 H ATOM 249 N GLY A 21144.445 4.680 8.089 1.00 0.00 N **ATOM** 250 CA GLY A 21143.912 3.996 9.253 1.00 0.00 C ATOM **ATOM** 251 C GLYA 21142.916 2.914 8.885 1.00 0.00 C 252 O GLY A 21142.848 1.876 9.542 1.00 0.00 O ATOM 253 H GLY A 21145.130 4.247 7.539 1.00 0.00 H ATOM 254 1HA GLY A 21144.730 3.548 9.799 1.00 0.00 H **ATOM** 255 2HA GLY A 21143.424 4.720 9.888 1.00 0.00 H **ATOM ATOM** 256 N SER A 22142.142 3.158 7.834 1.00 0.00 N 257 CA SER A 22141.145 2.196 7.379 1.00 0.00 C ATOM 258 C SER A 22141.791 1.093 6.546 1.00 0.00 C **ATOM** 259 O SER A 22142.817 1.309 5.902 1.00 0.00 O **ATOM** 260 CB SER A 22140.061 2.901 6.561 1.00 0.00 C **ATOM ATOM** 261 OG SER A 22139.134 3.563 7.404 1.00 0.00 O 262 H SER A 22142.245 4.005 7.350 1.00 0.00 H **ATOM** 263 HA SER A 22140.691 1.752 8.253 1.00 0.00 H **ATOM** 264 1HB SER A 22140.522 3.631 5.911 1.00 0.00 H **ATOM** 265 2HB SER A 22139.532 2.172 5.965 1.00 0.00 H ATOM 266 HG SER A 22139.608 4.049 8.083 1.00 0.00 H ATOM **ATOM** 267 N LEUA 23141.182 -0.088 6.563 1.00 0.00 N 268 CA LEU A 23141.698 -1.224 5.809 1.00 0.00 C ATOM 269 C LEUA 23141.307 -1.125 4.338 1.00 0.00 C **ATOM** 270 O LEUA 23140.274 -0.549 3.998 1.00 0.00 O **ATOM** 271 CB LEU A 23141.177 -2.535 6.399 1.00 0.00 C **ATOM** 272 CG LEU A 23141.354 -2.680 7.911 1.00 0.00 C ATOM ATOM 273 CD1 LEU A 23140.277 -3.584 8.491 1.00 0.00 C 274 CD2 LEU A 23142.738 -3.221 8.235 1.00 0.00 C ATOM 275 H LEUA 23140.367 -0.198 7.095 1.00 0.00 H **ATOM** ATOM 276 HA LEU A 23142.775 -1.210 5.884 1.00 0.00 H

277 1HB LEU A 23140.123 -2.612 6.172 1.00 0.00 H 278 2HB LEU A 23141.693 -3.352 5.919 1.00 0.00 H **ATOM** 279 HG LEU A 23141.257 -1.708 8.373 1.00 0.00 H 280 1HD1 LEU A 23140.028 -3.253 9.489 1.00 0.00 H **ATOM** 281 2HD1 LEU A 23140.642 -4.600 8.529 1.00 0.00 H **ATOM** 282 3HD1 LEU A 23139.396 -3.540 7.868 1.00 0.00 H **ATOM ATOM** 283 1HD2 LEU A 23143.421 -2.963 7.439 1.00 0.00 H **ATOM** 284 2HD2 LEU A 23142.691 -4.296 8.333 1.00 0.00 H **ATOM** 285 3HD2 LEU A 23143.085 -2.791 9.162 1.00 0.00 H **ATOM** 286 N ALAA 24142.140 -1.689 3.470 1.00 0.00 N 287 CA ALA A 24141.882 -1.663 2.035 1.00 0.00 C **ATOM** ATOM 288 C ALAA 24142.477 -2.887 1.349 1.00 0.00 C 289 O ALAA 24143.416 -3.502 1.856 1.00 0.00 O **ATOM** 290 CB ALAA 24142.439 -0.388 1.421 1.00 0.00 C **ATOM ATOM** 291 H ALAA 24142.948 -2.133 3.802 1.00 0.00 H **ATOM** 292 HA ALA A 24140.811 -1.667 1.890 1.00 0.00 H ATOM 293 1HB ALA A 24143.407 -0.591 0.986 1.00 0.00 H 294 2HB ALA A 24142.541 0.365 2.188 1.00 0.00 H **ATOM** 295 3HB ALAA 24141.767 -0.034 0.654 1.00 0.00 H **ATOM** 296 N GLUA 25141.926 -3.237 0.191 1.00 0.00 N ATOM 297 CA GLU A 25142.403 -4.388 -0.566 1.00 0.00 C **ATOM** 298 C GLU A 25142.632 -4.020 -2.029 1.00 0.00 C **ATOM** 299 O GLUA 25141.891 -3.223 -2.602 1.00 0.00 O ATOM 300 CB GLU A 25141.401 -5.540 -0.470 1.00 0.00 C **ATOM ATOM** 301 CG GLU A 25142.005 -6.899 -0.780 1.00 0.00 C 302 CD GLUA 25141.078 -7.776 -1.599 1.00 0.00 C **ATOM** 303 OE1 GLU A 25141.583 -8.664 -2.319 1.00 0.00 O **ATOM** 304 OE2 GLU A 25139.847 -7.577 -1.520 1.00 0.00 O ATOM 305 H GLUA 25141.181 -2.708 -0.163 1.00 0.00 H **ATOM** 306 HA GLU A 25143.341 -4.703 -0.135 1.00 0.00 H ATOM 307 1HB GLU A 25140.998 -5.569 0.532 1.00 0.00 H

- ATOM 308 2HB GLU A 25140.596 -5.360 -1.167 1.00 0.00 H
- ATOM 309 1HG GLU A 25142.920 -6.755 -1.332 1.00 0.00 H
- ATOM 310 2HG GLU A 25142.223 -7.402 0.152 1.00 0.00 H
- ATOM 311 N VALA 26143.664 -4.607 -2.627 1.00 0.00 N
- ATOM 312 CA VALA 26143.992 -4.340 -4.022 1.00 0.00 C
- ATOM 313 C VALA 26143.563 -5.497 -4.918 1.00 0.00 C
- ATOM 314 O VALA 26143.381 -6.622 -4.450 1.00 0.00 O
- ATOM 315 CB VALA 26145.500 -4.093 -4.208 1.00 0.00 C
- ATOM 316 CG1 VAL A 26145.793 -3.607 -5.619 1.00 0.00 C
- ATOM 317 CG2 VAL A 26146.010 -3.097 -3.177 1.00 0.00 C
- ATOM 318 H VALA 26144.220 -5.233 -2.117 1.00 0.00 H
- ATOM 319 HA VALA 26143.462 -3.448 -4.325 1.00 0.00 H
- ATOM 320 HB VAL A 26146.019 -5.029 -4.060 1.00 0.00 H
- ATOM 321 1HG1 VAL A 26145.913 -4.456 -6.276 1.00 0.00 H
- ATOM 322 2HG1 VAL A 26146.700 -3.022 -5.618 1.00 0.00 H
- ATOM 323 3HG1 VAL A 26144.972 -2.997 -5.968 1.00 0.00 H
- ATOM 324 1HG2 VAL A 26146.053 -3.572 -2.209 1.00 0.00 H
- ATOM 325 2HG2 VAL A 26145.341 -2.250 -3.133 1.00 0.00 H
- ATOM 326 3HG2 VAL A 26146.998 -2.762 -3.457 1.00 0.00 H
- ATOM 327 N LYS A 27143.402 -5.215 -6.206 1.00 0.00 N
- ATOM 328 CA LYS A 27142.994 -6.233 -7.167 1.00 0.00 C
- ATOM 329 C LYS A 27144.201 -6.795 -7.911 1.00 0.00 C
- ATOM 330 O LYS A 27144.125 -7.090 -9.103 1.00 0.00 O
- ATOM 331 CB LYS A 27141.991 -5.650 -8.164 1.00 0.00 C
- ATOM 332 CG LYS A 27142.567 -4.539 -9.028 1.00 0.00 C
- ATOM 333 CD LYS A 27141.949 -4.536 -10.418 1.00 0.00 C
- ATOM 334 CE LYS A 27142.791 -5.328 -11.406 1.00 0.00 C
- ATOM 335 NZ LYS A 27141.989 -6.363 -12.115 1.00 0.00 N
- ATOM 336 H LYS A 27143.561 -4.300 -6.518 1.00 0.00 H
- ATOM 337 HA LYS A 27142.519 -7.033 -6.620 1.00 0.00 H
- ATOM 338 1HB LYS A 27141.647 -6.440 -8.815 1.00 0.00 H

339 2HB LYS A 27141.149 -5.252 -7.619 1.00 0.00 H ATOM 340 1HG LYS A 27142.369 -3.589 -8.556 1.00 0.00 H ATOM 341 2HG LYS A 27143.634 -4.683 -9.117 1.00 0.00 H ATOM 342 1HD LYS A 27140.966 -4.979 -10.364 1.00 0.00 H ATOM 343 2HD LYS A 27141.868 -3.516 -10.762 1.00 0.00 H ATOM 344 1HE LYS A 27143.204 -4.646 -12.134 1.00 0.00 H **ATOM** 345 2HE LYS A 27143.595 -5.812 -10.871 1.00 0.00 H ATOM 346 1HZ LYS A 27142.045 -7.269 -11.606 1.00 0.00 H **ATOM** 347 2HZ LYS A 27142.351 -6.497 -13.081 1.00 0.00 H **ATOM** 348 3HZ LYS A 27140.993 -6.068 -12.168 1.00 0.00 H **ATOM** 349 N GLUA 28145.314 -6.940 -7.199 1.00 0.00 N ATOM 350 CA GLUA 28146.537 -7.467 -7.793 1.00 0.00 C **ATOM** ATOM 351 C GLUA 28146.479 -8.988 -7.899 1.00 0.00 C 352 O GLUA 28145.509 -9.614 -7.472 1.00 0.00 O ATOM 353 CB GLUA 28147.753 -7.046 -6.964 1.00 0.00 C ATOM 354 CG GLUA 28148.886 -6.467 -7.797 1.00 0.00 C ATOM 355 CD GLUA 28150.212 -6.475 -7.064 1.00 0.00 C **ATOM** 356 OE1 GLU A 28150.759 -5.379 -6.815 1.00 0.00 O ATOM 357 OE2 GLU A 28150.704 -7.575 -6.738 1.00 0.00 O ATOM 358 H GLUA 28145.312 -6.687 -6.252 1.00 0.00 H **ATOM** 359 HA GLU A 28146.628 -7.052 -8.786 1.00 0.00 H **ATOM** 360 1HB GLU A 28147.445 -6.299 -6.248 1.00 0.00 H ATOM 361 2HB GLU A 28148.131 -7.908 -6.433 1.00 0.00 H **ATOM** 362 1HG GLU A 28148.987 -7.052 -8.699 1.00 0.00 H **ATOM** 363 2HG GLU A 28148.639 -5.448 -8.058 1.00 0.00 H **ATOM** 364 N ASNA 29147.525 -9.576 -8.471 1.00 0.00 N **ATOM** 365 CA ASN A 29147.594 -11.024 -8.632 1.00 0.00 C **ATOM** 366 C ASN A 29147.522 -11.726 -7.277 1.00 0.00 C **ATOM** 367 O ASNA 29146.628 -12.537 -7.037 1.00 0.00 O **ATOM** 368 CB ASN A 29148.882 -11.416 -9.358 1.00 0.00 C **ATOM** 369 CG ASN A 29148.671 -11.604 -10.847 1.00 0.00 C ATOM

- ATOM 370 OD1 ASN A 29148.987 -12.657 -11.403 1.00 0.00 O
- ATOM 371 ND2 ASN A 29148.135 -10.581 -11.504 1.00 0.00 N
- ATOM 372 H ASN A 29148.269 -9.024 -8.791 1.00 0.00 H
- ATOM 373 HA ASN A 29146.747 -11.331 -9.228 1.00 0.00 H
- ATOM 374 1HB ASN A 29149.620 -10.641 -9.214 1.00 0.00 H
- ATOM 375 2HB ASN A 29149.253 -12.343 -8.946 1.00 0.00 H
- ATOM 376 1HD2 ASN A 29147.909 -9.774 -10.996 1.00 0.00 H
- ATOM 377 2HD2 ASN A 29147.987 -10.675 -12.468 1.00 0.00 H
- ATOM 378 N PRO A 30148.467 -11.421 -6.372 1.00 0.00 N
- ATOM 379 CA PRO A 30148.507 -12.026 -5.039 1.00 0.00 C
- ATOM 380 C PRO A 30147.460 -11.429 -4.099 1.00 0.00 C
- ATOM 381 O PRO A 30147.579 -10.276 -3.682 1.00 0.00 O
- ATOM 382 CB PRO A 30149.915 -11.691 -4.549 1.00 0.00 C
- ATOM 383 CG PRO A 30150.256 -10.414 -5.236 1.00 0.00 C
- ATOM 384 CD PRO A 30149.572 -10.463 -6.576 1.00 0.00 C
- ATOM 385 HA PRO A 30148.384 -13.098 -5.085 1.00 0.00 H
- ATOM 386 1HB PRO A 30149.908 -11.575 -3.475 1.00 0.00 H
- ATOM 387 2HB PRO A 30150.595 -12.482 -4.827 1.00 0.00 H
- ATOM 388 1HG PRO A 30149.888 -9.578 -4.658 1.00 0.00 H
- ATOM 389 2HG PRO A 30151.326 -10.340 -5.363 1.00 0.00 H
- ATOM 390 1HD PRO A 30149.191 -9.487 -6.840 1.00 0.00 H
- ATOM 391 2HD PRO A 30150.254 -10.817 -7.334 1.00 0.00 H
- ATOM 392 N PRO A 31146.417 -12.204 -3.751 1.00 0.00 N
- ATOM 393 CA PRO A 31145.353 -11.735 -2.857 1.00 0.00 C
- ATOM 394 C PRO A 31145.844 -11.540 -1.426 1.00 0.00 C
- ATOM 395 O PRO A 31145.741 -12.443 -0.595 1.00 0.00 O
- ATOM 396 CB PRO A 31144.313 -12.857 -2.917 1.00 0.00 C
- ATOM 397 CG PRO A 31145.088 -14.071 -3.297 1.00 0.00 C
- ATOM 398 CD PRO A 31146.191 -13.592 -4.199 1.00 0.00 C
- ATOM 399 HA PRO A 31144.914 -10.815 -3.213 1.00 0.00 H
- ATOM 400 1HB PRO A 31143.847 -12.973 -1.949 1.00 0.00 H

401 2HB PRO A 31143.565 -12.620 -3.658 1.00 0.00 H 402 1HG PRO A 31145.501 -14.535 -2.413 1.00 0.00 H ATOM 403 2HG PRO A 31144.449 -14.766 -3.823 1.00 0.00 H ATOM 404 1HD PRO A 31147.078 -14.192 -4.061 1.00 0.00 H **ATOM** 405 2HD PRO A 31145.872 -13.617 -5.230 1.00 0.00 H ATOM 406 N PHE A 32146.377 -10.356 -1.146 1.00 0.00 N ATOM 407 CA PHE A 32146.885 -10.041 0.185 1.00 0.00 C ATOM 408 C PHE A 32145.947 -9.083 0.912 1.00 0.00 C ATOM 409 O PHE A 32144.998 -8.562 0.324 1.00 0.00 O ATOM 410 CB PHE A 32148.283 -9.430 0.090 1.00 0.00 C ATOM 411 CG PHE A 32148.404 -8.366 -0.964 1.00 0.00 C ATOM 412 CD1 PHE A 32147.687 -7.185 -0.859 1.00 0.00 C 413 CD2 PHE A 32149.233 -8.548 -2.059 1.00 0.00 C **ATOM** 414 CE1 PHE A 32147.796 -6.205 -1.827 1.00 0.00 C ATOM 415 CE2 PHE A 32149.346 -7.572 -3.030 1.00 0.00 C ATOM 416 CZ PHE A 32148.626 -6.397 -2.914 1.00 0.00 C ATOM 417 H PHE A 32146.430 -9.677 -1.850 1.00 0.00 H ATOM 418 HA PHE A 32146.941 -10.963 0.744 1.00 0.00 H **ATOM** 419 1HB PHE A 32148.540 -8.987 1.040 1.00 0.00 H **ATOM** 420 2HB PHE A 32148.994 -10.210 -0.141 1.00 0.00 H **ATOM** 421 HD1 PHE A 32147.038 -7.032 -0.010 1.00 0.00 H ATOM 422 HD2 PHE A 32149.796 -9.465 -2.151 1.00 0.00 H **ATOM** 423 HE1 PHE A 32147.232 -5.289 -1.734 1.00 0.00 H ATOM 424 HE2 PHE A 32149.995 -7.724 -3.879 1.00 0.00 H ATOM 425 HZ PHE A 32148.712 -5.632 -3.672 1.00 0.00 H ATOM 426 N TYR A 33146.217 -8.856 2.193 1.00 0.00 N ATOM 427 CA TYR A 33145.397 -7.958 2.999 1.00 0.00 C ATOM 428 C TYR A 33146.269 -6.990 3.793 1.00 0.00 C ATOM 429 O TYR A 33147.270 -7.387 4.389 1.00 0.00 O ATOM 430 CB TYR A 33144.511 -8.763 3.952 1.00 0.00 C **ATOM** 431 CG TYR A 33143.249 -9.290 3.306 1.00 0.00 C ATOM

432 CD1 TYR A 33142.903 -10.632 3,406 1.00 0.00 C ATOM 433 CD2 TYR A 33142.405 -8.447 2.595 1.00 0.00 C 434 CE1 TYR A 33141.751 -11.118 2.817 1.00 0.00 C ATOM 435 CE2 TYR A 33141.251 -8.925 2.003 1.00 0.00 C ATOM 436 CZ TYR A 33140.929 -10.261 2.116 1.00 0.00 C ATOM ATOM 437 OH TYR A 33139.781 -10.740 1.529 1.00 0.00 O 438 H TYR A 33146.987 -9.300 2.605 1.00 0.00 H ATOM 439 HA TYR A 33144.769 -7.392 2.329 1.00 0.00 H ATOM 440 1HB TYR A 33145.069 -9.608 4.325 1.00 0.00 H **ATOM ATOM** 441 2HB TYR A 33144.222 -8.134 4.780 1.00 0.00 H ATOM 442 HD1 TYR A 33143.549 -11.302 3.956 1.00 0.00 H ATOM 443 HD2 TYR A 33142.661 -7.401 2.507 1.00 0.00 H 444 HE1 TYR A 33141.500 -12.165 2.907 1.00 0.00 H ATOM 445 HE2 TYR A 33140.609 -8.253 1.455 1.00 0.00 H ATOM 446 HH TYR A 33139.736 -10.436 0.620 1.00 0.00 H **ATOM** 447 N GLY A 34145.880 -5.719 3.796 1.00 0.00 N ATOM 448 CA GLY A 34146.637 -4.715 4.519 1.00 0.00 C ATOM 449 C GLY A 34145.778 -3.546 4.957 1.00 0.00 C **ATOM** 450 O GLY A 34144.551 -3.643 4.984 1.00 0.00 O ATOM 451 H GLY A 34145.074 -5.462 3.302 1.00 0.00 H ATOM 452 1HA GLY A 34147.077 -5.172 5.393 1.00 0.00 H **ATOM** 453 2HA GLY A 34147.427 -4.348 3.881 1.00 0.00 H **ATOM ATOM** 454 N VALA 35146.423 -2.435 5.301 1.00 0.00 N 455 CA VALA 35145.710 -1.242 5.740 1.00 0.00 C ATOM 456 C VALA 35146.363 0.022 5.187 1.00 0.00 C ATOM 457 O VALA 35147.577 0.070 4.991 1.00 0.00 O ATOM 458 CB VALA 35145.657 -1.154 7.279 1.00 0.00 C ATOM 459 CG1 VAL A 35147.060 -1.060 7.861 1.00 0.00 C ATOM 460 CG2 VAL A 35144.809 0.029 7.720 1.00 0.00 C ATOM 461 H VALA 35147.402 -2.420 5.259 1.00 0.00 H ATOM ATOM 462 HA VALA 35144.698 -1.304 5.370 1.00 0.00 H

ATOM 463 HB VALA 35145.199 -2.057 7.654 1.00 0.00 H 464 1HG1 VAL A 35147.690 -1.812 7.406 1.00 0.00 H **ATOM** ATOM 465 2HG1 VAL A 35147.020 -1.222 8.927 1.00 0.00 H 466 3HG1 VAL A 35147.468 -0.080 7.660 1.00 0.00 H ATOM 467 1HG2 VAL A 35143.784 -0.133 7.423 1.00 0.00 H ATOM ATOM 468 2HG2 VAL A 35145.180 0.932 7.257 1.00 0.00 H ATOM 469 3HG2 VAL A 35144.861 0.129 8.795 1.00 0.00 H ATOM 470 N ILE A 36145.548 1.042 4.939 1.00 0.00 N 471 CA ILE A 36146.046 2.306 4.409 1.00 0.00 C **ATOM** 472 C ILE A 36146.970 2.992 5.410 1.00 0.00 C ATOM ATOM 473 O ILE A 36146.688 3.027 6.607 1.00 0.00 O ATOM 474 CB ILE A 36144.891 3.262 4.051 1.00 0.00 C ATOM 475 CG1 ILE A 36143.876 2.558 3.149 1.00 0.00 C **ATOM** 476 CG2 ILE A 36145.430 4.514 3.374 1.00 0.00 C 477 CD1 ILE A 36142.709 3.435 2.752 1.00 0.00 C ATOM 478 H ILE A 36144.590 0.943 5.117 1.00 0.00 H **ATOM** ATOM 479 HA ILE A 36146.603 2.093 3.508 1.00 0.00 H ATOM 480 HB ILE A 36144.404 3.561 4.967 1.00 0.00 H 481 1HG1 ILE A 36144.369 2.234 2.246 1.00 0.00 H ATOM 482 2HG1 ILE A 36143.482 1.695 3.667 1.00 0.00 H ATOM 483 1HG2 ILE A 36146.162 4.235 2.630 1.00 0.00 H ATOM **ATOM** 484 2HG2 ILE A 36145.893 5.152 4.112 1.00 0.00 H 485 3HG2 ILE A 36144.618 5.044 2.898 1.00 0.00 H ATOM 486 1HD1 ILE A 36142.535 3.343 1.690 1.00 0.00 H ATOM 487 2HD1 ILE A 36142.935 4.464 2.992 1.00 0.00 H ATOM 488 3HD1 ILE A 36141.826 3.126 3.290 1.00 0.00 H ATOM **ATOM** 489 N ARGA 37148.076 3.535 4.910 1.00 0.00 N 490 CA ARG A 37149.042 4.220 5.761 1.00 0.00 C ATOM 491 C ARG A 37149.240 5.664 5.308 1.00 0.00 C ATOM 492 O ARG A 37148.974 6.601 6.060 1.00 0.00 O ATOM ATOM 493 CB ARG A 37150.382 3.480 5.742 1.00 0.00 C

494 CG ARG A 37150.258 1.992 6.024 1.00 0.00 C ATOM 495 CD ARG A 37149.607 1.733 7.373 1.00 0.00 C ATOM 496 NE ARG A 37150.302 2.420 8.458 1.00 0.00 N **ATOM** 497 CZ ARG A 37149.765 2.653 9.653 1.00 0.00 C ATOM 498 NH1 ARG A 37148.527 2.255 9.921 1.00 0.00 N **ATOM** 499 NH2 ARG A 37150.467 3.285 10.584 1.00 0.00 N ATOM 500 H ARG A 37148.246 3.474 3.947 1.00 0.00 H ATOM 501 HA ARG A 37148.656 4.221 6.768 1.00 0.00 H ATOM 502 1HB ARG A 37150.835 3.605 4.769 1.00 0.00 H **ATOM ATOM** 503 2HB ARG A 37151.030 3.914 6.489 1.00 0.00 H 504 1HG ARG A 37149.657 1.537 5.251 1.00 0.00 H **ATOM** 505 2HG ARG A 37151.245 1.553 6.020 1.00 0.00 H **ATOM** 506 1HD ARG A 37148.585 2.079 7.337 1.00 0.00 H **ATOM** 507 2HD ARG A 37149.620 0.670 7.565 1.00 0.00 H **ATOM** 508 HE ARG A 37151.219 2.724 8.288 1.00 0.00 H **ATOM** 509 1HH1 ARG A 37147.992 1.778 9.224 1.00 0.00 H ATOM 510 2HH1 ARG A 37148.129 2.432 10.820 1.00 0.00 H **ATOM** 511 1HH2 ARG A 37151.400 3.585 10.387 1.00 0.00 H ATOM 512 2HH2 ARG A 37150.063 3.460 11.482 1.00 0.00 H ATOM 513 N TRPA 38149.705 5.835 4.075 1.00 0.00 N ATOM 514 CA TRP A 38149.938 7.166 3.525 1.00 0.00 C ATOM 515 C TRPA 38149.254 7.323 2.169 1.00 0.00 C ATOM 516 O TRPA 38149.360 6.454 1.304 1.00 0.00 O **ATOM** 517 CB TRPA 38151.441 7.431 3.388 1.00 0.00 C ATOM 518 CG TRP A 38151.763 8.666 2.600 1.00 0.00 C ATOM 519 CD1 TRP A 38151.926 9.931 3.086 1.00 0.00 C ATOM 520 CD2 TRP A 38151.955 8.752 1.183 1.00 0.00 C ATOM 521 NE1 TRP A 38152.207 10.799 2.058 1.00 0.00 N ATOM 522 CE2 TRP A 38152.231 10.098 0.880 1.00 0.00 C ATOM 523 CE3 TRP A 38151.921 7.821 0.141 1.00 0.00 C ATOM ATOM 524 CZ2 TRP A 38152.471 10.535 -0.422 1.00 0.00 C

ATOM 525 CZ3 TRP A 38152.159 8.254 -1.149 1.00 0.00 C 526 CH2 TRP A 38152.431 9.601 -1.420 1.00 0.00 C **ATOM** ATOM 527 H TRP A 38149.898 5.049 3.523 1.00 0.00 H 528 HA TRP A 38149.516 7.885 4.211 1.00 0.00 H ATOM 529 1HB TRP A 38151.871 7.544 4.373 1.00 0.00 H **ATOM** 530 2HB TRP A 38151.904 6.589 2.894 1.00 0.00 H ATOM 531 HD1 TRP A 38151.842 10.198 4.129 1.00 0.00 H **ATOM** 532 HE1 TRP A 38152.366 11.761 2.153 1.00 0.00 H **ATOM** 533 HE3 TRP A 38151.713 6.779 0.331 1.00 0.00 H **ATOM** 534 HZ2 TRP A 38152.679 11.570 -0.648 1.00 0.00 H ATOM 535 HZ3 TRP A 38152.138 7.548 -1.966 1.00 0.00 H ATOM ATOM 536 HH2 TRP A 38152.612 9.895 -2.444 1.00 0.00 H ATOM 537 N ILE A 39148.559 8.442 1.993 1.00 0.00 N ATOM 538 CA ILE A 39147.864 8.725 0.744 1.00 0.00 C ATOM 539 C ILE A 39148.314 10.064 0.170 1.00 0.00 C ATOM 540 O ILE A 39147.947 11.122 0.681 1.00 0.00 O ATOM 541 CB ILE A 39146.337 8.750 0.942 1.00 0.00 C ATOM 542 CG1 ILE A 39145.876 7.502 1.698 1.00 0.00 C 543 CG2 ILE A 39145.630 8.855 -0.400 1.00 0.00 C ATOM 544 CD1 ILE A 39144.499 7.639 2.309 1.00 0.00 C **ATOM** 545 H ILEA 39148.519 9.097 2.721 1.00 0.00 H **ATOM** 546 HA ILE A 39148.104 7.941 0.041 1.00 0.00 H **ATOM** ATOM 547 HB ILE A 39146.085 9.626 1.522 1.00 0.00 H 548 1HG1 ILE A 39145.854 6.665 1.016 1.00 0.00 H **ATOM** 549 2HG1 ILE A 39146.575 7.294 2.494 1.00 0.00 H ATOM ATOM 550 1HG2 ILE A 39146.098 9.626 -0.994 1.00 0.00 H ATOM 551 2HG2 ILE A 39144.590 9.104 -0.243 1.00 0.00 H 552 3HG2 ILE A 39145.699 7.909 -0.918 1.00 0.00 H ATOM ATOM 553 1HD1 ILE A 39144.001 8.499 1.886 1.00 0.00 H ATOM 554 2HD1 ILE A 39144.590 7.764 3.378 1.00 0.00 H ATOM 555 3HD1 ILE A 39143.922 6.750 2.099 1.00 0.00 H

556 N GLYA 40149.115 10.011 -0.889 1.00 0.00 N ATOM 557 CA GLY A 40149.604 11.231 -1.504 1.00 0.00 C **ATOM** 558 C GLYA 40150.212 10.994 -2.873 1.00 0.00 C ATOM 559 O GLYA 40150.068 9.916 -3.447 1.00 0.00 O ATOM 560 H GLY A 40149.379 9.141 -1.252 1.00 0.00 H ATOM 561 1HA GLY A 40148.785 11.925 -1.603 1.00 0.00 H ATOM ATOM 562 2HA GLY A 40150.353 11.667 -0.862 1.00 0.00 H 563 N GLN A 41150.892 12.010 -3.394 1.00 0.00 N **ATOM** 564 CA GLN A 41151.525 11.919 -4.703 1.00 0.00 C **ATOM** 565 C GLNA 41153.000 12.311 -4.618 1.00 0.00 C ATOM 566 O GLN A 41153.325 13.461 -4.321 1.00 0.00 O **ATOM** 567 CB GLN A 41150.799 12.825 -5.696 1.00 0.00 C **ATOM** 568 CG GLN A 41149.288 12.653 -5.685 1.00 0.00 C ·ATOM 569 CD GLN A 41148.551 13.969 -5.825 1.00 0.00 C **ATOM** 570 OE1 GLN A 41148.474 14.755 -4.881 1.00 0.00 O **ATOM** 571 NE2 GLN A 41148.004 14.216 -7.009 1.00 0.00 N ATOM 572 H GLN A 41150.968 12.844 -2.886 1.00 0.00 H **ATOM** 573 HA GLN A 41151.451 10.897 -5.040 1.00 0.00 H **ATOM** 574 1HB GLN A 41151.023 13.853 -5.456 1.00 0.00 H **ATOM** 575 2HB GLN A 41151.158 12.610 -6.690 1.00 0.00 H **ATOM** 576 1HG GLN A 41149.005 12.010 -6.504 1.00 0.00 H ATOM 577 2HG GLN A 41148.999 12.192 -4.752 1.00 0.00 H **ATOM** 578 1HE2 GLN A 41148.106 13.544 -7.715 1.00 0.00 H **ATOM** 579 2HE2 GLN A 41147.522 15.061 -7.130 1.00 0.00 H **ATOM** 580 N PRO A 42153.917 11.361 -4.876 1.00 0.00 N **ATOM** 581 CA PRO A 42155.360 11.623 -4.822 1.00 0.00 C ATOM 582 C PRO A 42155.779 12.746 -5.766 1.00 0.00 C ATOM 583 O PROA 42155.066 13.071 -6.715 1.00 0.00 O ATOM 584 CB PRO A 42155.986 10.295 -5.261 1.00 0.00 C **ATOM** 585 CG PRO A 42154.937 9.272 -5.000 1.00 0.00 C **ATOM** 586 CD PRO A 42153.626 9.962 -5.237 1.00 0.00 C **ATOM**

587 HA PRO A 42155.680 11.861 -3.819 1.00 0.00 H ATOM 588 1HB PRO A 42156.239 10.344 -6.311 1.00 0.00 H **ATOM ATOM** 589 2HB PRO A 42156.877 10.105 -4.680 1.00 0.00 H 590 1HG PRO A 42155.053 8.442 -5.681 1.00 0.00 H ATOM **ATOM** 591 2HG PRO A 42155.002 8.931 -3.976 1.00 0.00 H 592 1HD PRO A 42153.340 9.882 -6.276 1.00 0.00 H **ATOM ATOM** 593 2HD PRO A 42152.859 9.550 -4.598 1.00 0.00 H **ATOM** 594 N PRO A 43156.951 13.355 -5.515 1.00 0.00 N **ATOM** 595 CA PRO A 43157.466 14.446 -6.347 1.00 0.00 C **ATOM** 596 C PRO A 43157.941 13.958 -7.711 1.00 0.00 C **ATOM** 597 O PRO A 43159.115 13.636 -7.891 1.00 0.00 O **ATOM** 598 CB PRO A 43158.643 14.986 -5.535 1.00 0.00 C 599 CG PRO A 43159.098 13.830 -4.714 1.00 0.00 C ATOM 600 CD PRO A 43157.863 13.027 -4.403 1.00 0.00 C **ATOM ATOM** 601 HA PRO A 43156.729 15.225 -6.481 1.00 0.00 H 602 1HB PRO A 43159.419 15.323 -6.207 1.00 0.00 H ATOM 603 2HB PRO A 43158.312 15.805 -4.915 1.00 0.00 H ATOM 604 1HG PRO A 43159.800 13.233 -5.277 1.00 0.00 H **ATOM** 605 2HG PRO A 43159.553 14.185 -3.800 1.00 0.00 H ATOM 606 1HD PRO A 43158.092 11.973 -4.391 1.00 0.00 H **ATOM** 607 2HD PRO A 43157.442 13.334 -3.457 1.00 0.00 H **ATOM** 608 N GLY A 44157.022 13.906 -8.667 1.00 0.00 N **ATOM** 609 CA GLY A 44157.369 13.457 -10.002 1.00 0.00 C **ATOM** 610 C GLY A 44156.170 12.942 -10.771 1.00 0.00 C ATOM 611 O GLY A 44155.925 13.359 -11.903 1.00 0.00 O ATOM 612 H GLY A 44156.101 14.175 -8.467 1.00 0.00 H ATOM 613 1HA GLY A 44157.804 14.281 -10.546 1.00 0.00 H ATOM 614 2HA GLY A 44158.100 12.664 -9.924 1.00 0.00 H ATOM 615 N LEUA 45155.420 12.034 -10.156 1.00 0.00 N **ATOM** 616 CA LEU A 45154.240 11.463 -10.793 1.00 0.00 C ATOM ATOM 617 C LEU A 45152.994 11.726 -9.956 1.00 0.00 C

618 O LEUA 45152.847 11.184 -8.860 1.00 0.00 O 619 CB LEUA 45154.422 9.959 -10.999 1.00 0.00 C **ATOM** 620 CG LEUA 45154.906 9.191 -9.766 1.00 0.00 C **ATOM** 621 CD1 LEU A 45154.533 7.718 -9.873 1.00 0.00 C **ATOM** 622 CD2 LEU A 45156.411 9.354 -9.592 1.00 0.00 C ATOM 623 H LEUA 45155.664 11.743 -9.251 1.00 0.00 H ATOM ATOM 624 HA LEUA 45154.119 11.938 -11.754 1.00 0.00 H 625 1HB LEU A 45153.476 9.542 -11.310 1.00 0.00 H ATOM 626 2HB LEU A 45155.140 9.810 -11.791 1.00 0.00 H **ATOM** 627 HG LEU A 45154.421 9.594 -8.889 1.00 0.00 H **ATOM** 628 1HD1 LEU A 45155.414 7.111 -9.728 1.00 0.00 H **ATOM ATOM** 629 2HD1 LEU A 45154.117 7.521 -10.849 1.00 0.00 H 630 3HD1 LEU A 45153.803 7.477 -9.114 1.00 0.00 H **ATOM** 631 1HD2 LEU A 45156.770 10.126 -10.257 1.00 0.00 H ATOM 632 2HD2 LEU A 45156.904 8.422 -9.824 1.00 0.00 H ATOM 633 3HD2 LEU A 45156.626 9.631 -8.571 1.00 0.00 H ATOM 634 N ASN A 46152.096 12.558 -10.474 1.00 0.00 N **ATOM** 635 CA ASN A 46150.868 12.879 -9.761 1.00 0.00 C ATOM 636 C ASN A 46149.905 11.697 -9.796 1.00 0.00 C ATOM 637 O ASN A 46149.319 11.390 -10.834 1.00 0.00 O **ATOM** 638 CB ASN A 46150.205 14.113 -10.378 1.00 0.00 C ATOM 639 CG ASN A 46149.419 14.917 -9.361 1.00 0.00 C ATOM **ATOM** 640 OD1 ASN A 46148.199 15.047 -9.464 1.00 0.00 O 641 ND2 ASN A 46150.117 15.463 -8.372 1.00 0.00 N **ATOM** 642 H ASN A 46152.264 12.961 -11.350 1.00 0.00 H **ATOM** 643 HA ASN A 46151.123 13.092 -8.733 1.00 0.00 H ATOM 644 1HB ASN A 46150.967 14.749 -10.800 1.00 0.00 H ATOM 645 2HB ASN A 46149.530 13.797 -11.160 1.00 0.00 H ATOM 646 1HD2 ASN A 46151.086 15.318 -8.353 1.00 0.00 H ATOM 647 2HD2 ASN A 46149.634 15.989 -7.700 1.00 0.00 H ATOM ATOM 648 N GLUA 47149.747 11.040 -8.654 1.00 0.00 N

649 CA GLU A 47148.857 9.891 -8.546 1.00 0.00 C ATOM 650 C GLUA 47148.612 9.532 -7.084 1.00 0.00 C **ATOM** 651 O GLUA 47149.551 9.232 -6.346 1.00 0.00 O **ATOM ATOM** 652 CB GLU A 47149.445 8.687 -9.288 1.00 0.00 C 653 CG GLU A 47150.953 8.556 -9.150 1.00 0.00 C ATOM 654 CD GLU A 47151.556 7.633 -10.192 1.00 0.00 C ATOM 655 OE1 GLU A 47151.850 6.467 -9.853 1.00 0.00 O ATOM 656 OE2 GLU A 47151.731 8.076 -11.347 1.00 0.00 O ATOM 657 H GLUA 47150.243 11.335 -7.862 1.00 0.00 H ATOM 658 HA GLU A 47147.916 10.158 -9.000 1.00 0.00 H ATOM 659 1HB GLU A 47148.991 7.786 -8.902 1.00 0.00 H ATOM 660 2HB GLU A 47149.208 8.776 -10.338 1.00 0.00 H ATOM **ATOM** 661 1HG GLU A 47151.398 9.534 -9.258 1.00 0.00 H 662 2HG GLU A 47151.182 8.166 -8.169 1.00 0.00 H ATOM 663 N VALA 48147.351 9.557 -6.671 1.00 0.00 N **ATOM** 664 CA VALA 48146.997 9.226 -5.298 1.00 0.00 C ATOM 665 C VALA 48147.343 7.775 -4.989 1.00 0.00 C ATOM 666 O VALA 48146.591 6.861 -5.329 1.00 0.00 O ATOM 667 CB VAL A 48145.499 9.456 -5.029 1.00 0.00 C ATOM 668 CG1 VALA 48145.192 9.299 -3.547 1.00 0.00 C ATOM 669 CG2 VAL A 48145.072 10.828 -5.527 1.00 0.00 C **ATOM** 670 H VALA 48146.643 9.799 -7.304 1.00 0.00 H **ATOM** 671 HA VALA 48147.567 9.869 -4.641 1.00 0.00 H **ATOM ATOM** 672 HB VALA 48144.938 8.708 -5.570 1.00 0.00 H 673 1HG1 VAL A 48144.163 9.571 -3.362 1.00 0.00 H ATOM

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674 2HG1 VAL A 48145.843 9.943 -2.974 1.00 0.00 H

675 3HG1 VAL A 48145.351 8.273 -3.252 1.00 0.00 H

676 1HG2 VAL A 48144.130 11.099 -5.073 1.00 0.00 H

677 2HG2 VAL A 48144.958 10.801 -6.601 1.00 0.00 H

678 3HG2 VAL A 48145.822 11.558 -5.263 1.00 0.00 H

ATOM 679 N LEUA 49148.487 7.569 -4.345 1.00 0.00 N

ATOM

ATOM

ATOM

ATOM

ATOM

680 CA LEU A 49148.934 6.227 -3.994 1.00 0.00 C **ATOM** 681 C LEUA 49148.788 5.983 -2.498 1.00 0.00 C ATOM ATOM 682 O LEUA 49149.449 6.633 -1.687 1.00 0.00 O 683 CB LEUA 49150.390 6.023 -4.417 1.00 0.00 C ATOM 684 CG LEUA 49150.667 6.237 -5.906 1.00 0.00 C **ATOM** 685 CD1 LEU A 49152.113 6.656 -6.125 1.00 0.00 C **ATOM ATOM** 686 CD2 LEU A 49150.352 4.974 -6.693 1.00 0.00 C 687 H LEUA 49149.045 8.336 -4.102 1.00 0.00 H **ATOM** 688 HA LEUA 49148.313 5.521 -4.524 1.00 0.00 H ATOM 689 1HB LEU A 49151.005 6.711 -3.855 1.00 0.00 H **ATOM ATOM** 690 2HB LEU A 49150.680 5.015 -4.162 1.00 0.00 H ATOM 691 HG LEU A 49150.032 7.029 -6.275 1.00 0.00 H ATOM 692 1HD1 LEU A 49152.177 7.734 -6.140 1.00 0.00 H **ATOM** 693 2HD1 LEU A 49152.464 6.261 -7.067 1.00 0.00 H 694 3HD1 LEU A 49152.725 6.271 -5.323 1.00 0.00 H ATOM 695 1HD2 LEU A 49151.242 4.367 -6.770 1.00 0.00 H ATOM 696 2HD2 LEU A 49150.012 5.241 -7.682 1.00 0.00 H ATOM **ATOM** 697 3HD2 LEU A 49149.579 4.416 -6.185 1.00 0.00 H 698 N ALAA 50147.919 5.047 -2.139 1.00 0.00 N ATOM 699 CA ALAA 50147.689 4.724 -0.738 1.00 0.00 C **ATOM** 700 C ALAA 50148.600 3.591 -0.281 1.00 0.00 C **ATOM** 701 O ALAA 50148.489 2.461 -0.758 1.00 0.00 O **ATOM** 702 CB ALAA 50146.230 4.357 -0.514 1.00 0.00 C ATOM **ATOM** 703 H ALAA 50147.421 4.564 -2.831 1.00 0.00 H 704 HA ALAA 50147.909 5.608 -0.156 1.00 0.00 H ATOM 705 1HB ALA A 50145.901 4.754 0.435 1.00 0.00 H **ATOM ATOM** 706 2HB ALA A 50146.126 3.282 -0.509 1.00 0.00 H 707 3HB ALAA 50145.628 4.775 -1.307 1.00 0.00 H ATOM **ATOM** 708 N GLYA 51149.502 3.899 0.645 1.00 0.00 N 709 CA GLY A 51150.420 2.895 1.151 1.00 0.00 C ATOM ATOM 710 C GLY A 51149.722 1.838 1.983 1.00 0.00 C

711 O GLYA 51149.241 2.120 3.081 1.00 0.00 O 712 H GLYA 51149.545 4.816 0.988 1.00 0.00 H **ATOM** 713 1HA GLY A 51150.907 2.415 0.315 1.00 0.00 H ATOM 714 2HA GLY A 51151.168 3.381 1.759 1.00 0.00 H ATOM 715 N LEUA 52149.667 0.617 1.461 1.00 0.00 N ATOM 716 CA LEU A 52149.023 -0.486 2.164 1.00 0.00 C **ATOM** ATOM 717 C LEUA 52150.052 -1.340 2.897 1.00 0.00 C 718 O LEUA 52151.062 -1.744 2.320 1.00 0.00 O ATOM 719 CB LEU A 52148.231 -1.352 1.183 1.00 0.00 C **ATOM** 720 CG LEU A 52146.974 -0.695 0.609 1.00 0.00 C ATOM 721 CD1 LEU A 52146.452 -1.490 -0.579 1.00 0.00 C **ATOM** 722 CD2 LEU A 52145.903 -0.569 1.680 1.00 0.00 C ATOM 723 H LEUA 52150.068 0.453 0.582 1.00 0.00 H ATOM 724 HA LEU A 52148.342 -0.064 2.889 1.00 0.00 H **ATOM** 725 1HB LEU A 52148.882 -1.616 0.362 1.00 0.00 H **ATOM** ATOM 726 2HB LEU A 52147.935 -2.258 1.692 1.00 0.00 H **ATOM** 727 HG LEU A 52147.222 0.298 0.262 1.00 0.00 H 728 1HD1 LEU A 52145.685 -2.174 -0.246 1.00 0.00 H **ATOM** 729 2HD1 LEU A 52147.263 -2.047 -1.023 1.00 0.00 H **ATOM ATOM** 730 3HD1 LEU A 52146.037 -0.812 -1.311 1.00 0.00 H 731 1HD2 LEU A 52145.344 0.343 1.526 1.00 0.00 H **ATOM** 732 2HD2 LEU A 52146.368 -0.544 2.655 1.00 0.00 H **ATOM** 733 3HD2 LEU A 52145.234 -1.414 1.622 1.00 0.00 H **ATOM** 734 N GLUA 53149.790 -1.612 4.171 1.00 0.00 N **ATOM** 735 CA GLUA 53150.694 -2.418 4.983 1.00 0.00 C ATOM 736 C GLU A 53150.200 -3.859 5.076 1.00 0.00 C ATOM 737 O GLUA 53149,205 -4.142 5.744 1.00 0.00 O ATOM **ATOM** 738 CB GLU A 53150.826 -1.819 6.384 1.00 0.00 C 739 CG GLU A 53151.783 -2.584 7.284 1.00 0.00 C ATOM 740 CD GLUA 53151.317 -2.629 8.726 1.00 0.00 C ATOM 741 OE1 GLU A 53151.200 -1.550 9.345 1.00 0.00 O ATOM

742 OE2 GLU A 53151.071 -3.742 9.236 1.00 0.00 O **ATOM** 743 H GLU A 53148.969 -1.262 4.575 1.00 0.00 H **ATOM** 744 HA GLU A 53151.662 -2.413 4.505 1.00 0.00 H **ATOM ATOM** 745 1HB GLU A 53151.182 -0.804 6.297 1.00 0.00 H 746 2HB GLU A 53149.854 -1.812 6.853 1.00 0.00 H ATOM 747 1HG GLU A 53151.870 -3.597 6.919 1.00 0.00 H ATOM 748 2HG GLUA 53152.751 -2.105 7.248 1.00 0.00 H ATOM 749 N LEUA 54150.903 -4.765 4.405 1.00 0.00 N ATOM 750 CA LEU A 54150.537 -6.176 4.412 1.00 0.00 C **ATOM** 751 C LEUA 54150.705 -6.775 5.805 1.00 0.00 C **ATOM** 752 O LEUA 54151.577 -6.360 6.568 1.00 0.00 O **ATOM** 753 CB LEU A 54151.389 -6.950 3.404 1.00 0.00 C ATOM **ATOM** 754 CG LEU A 54151.447 -6.342 2.002 1.00 0.00 C ATOM 755 CD1 LEU A 54152.766 -6.680 1.327 1.00 0.00 C 756 CD2 LEU A 54150.276 -6.829 1.162 1.00 0.00 C ATOM 757 H LEUA 54151.686 -4.477 3.891 1.00 0.00 H ATOM **ATOM** 758 HA LEU A 54149.498 -6.250 4.124 1.00 0.00 H 759 1HB LEU A 54152.396 -7.013 3.790 1.00 0.00 H ATOM 760 2HB LEU A 54150.990 -7.951 3.321 1.00 0.00 H ATOM 761 HG LEU A 54151.378 -5.266 2.081 1.00 0.00 H ATOM 762 1HD1 LEU A 54153.136 -7.620 1.710 1.00 0.00 H **ATOM** 763 2HD1 LEU A 54153.485 -5.901 1.531 1.00 0.00 H ATOM 764 3HD1 LEU A 54152.615 -6.761 0.261 1.00 0.00 H **ATOM** 765 1HD2 LEU A 54149.455 -7.099 1.811 1.00 0.00 H ATOM 766 2HD2 LEU A 54150.578 -7.692 0.589 1.00 0.00 H **ATOM** 767 3HD2 LEU A 54149.962 -6.043 0.492 1.00 0.00 H ATOM 768 N GLUA 55149.864 -7.752 6.128 1.00 0.00 N **ATOM** 769 CA GLU A 55149.920 -8.408 7.429 1.00 0.00 C **ATOM** 770 C GLUA 55151.075 -9.402 7.489 1.00 0.00 C ATOM ATOM 771 O GLUA 55151.677 -9.606 8.543 1.00 0.00 O ATOM 772 CB GLU A 55148.600 -9.124 7.719 1.00 0.00 C

773 CG GLU A 55147.559 -8.237 8.381 1.00 0.00 C **ATOM** 774 CD GLUA 55146.145 -8.576 7.952 1.00 0.00 C **ATOM** 775 OE1 GLU A 55145.281 -7.675 7.989 1.00 0.00 O **ATOM** 776 OE2 GLU A 55145.902 -9.743 7.576 1.00 0.00 O **ATOM** 777 H GLUA 55149.191 -8.038 5.477 1.00 0.00 H **ATOM** 778 HA GLUA 55150.077 -7.646 8.178 1.00 0.00 H **ATOM** ATOM 779 1HB GLUA 55148.191 -9.491 6.789 1.00 0.00 H 780 2HB GLU A 55148.794 -9.962 8.371 1.00 0.00 H **ATOM** 781 1HG GLUA 55147.631 -8.356 9.452 1.00 0.00 H **ATOM** 782 2HG GLU A 55147.762 -7.209 8.120 1.00 0.00 H **ATOM** 783 N ASPA 56151.380 -10.017 6.351 1.00 0.00 N **ATOM ATOM** 784 CA ASPA 56152.464 -10.989 6.275 1.00 0.00 C 785 C ASP A 56153.720 -10.358 5.682 1.00 0.00 C **ATOM** 786 O ASPA 56153.639 -9.461 4.844 1.00 0.00 O ATOM 787 CB ASPA 56152.038 -12.194 5.434 1.00 0.00 C **ATOM** 788 CG ASP A 56152.656 -13.489 5.924 1.00 0.00 C ATOM 789 OD1 ASPA 56151.930 -14.502 5.999 1.00 0.00 O ATOM 790 OD2 ASP A 56153.866 -13.489 6.233 1.00 0.00 O ATOM 791 H ASPA 56150.865 -9.811 5.544 1.00 0.00 H ATOM 792 HA ASP A 56152.682 -11.322 7.278 1.00 0.00 H **ATOM** 793 1HB ASPA 56150.963 -12.292 5.474 1.00 0.00 H ATOM 794 2HB ASPA 56152.343 -12.036 4.409 1.00 0.00 H **ATOM** 795 N GLUA 57154.880 -10.835 6.122 1.00 0.00 N ATOM 796 CA GLUA 57156.153 -10.318 5.635 1.00 0.00 C **ATOM** 797 C GLUA 57156.464 -10.862 4.244 1.00 0.00 C ATOM 798 O GLUA 57157.189 -11.845 4.098 1.00 0.00 O ATOM 799 CB GLU A 57157.281 -10.684 6.601 1.00 0.00 C ATOM 800 CG GLUA 57157.059 -10.172 8.016 1.00 0.00 C **ATOM** 801 CD GLU A 57156.643 -11.271 8.975 1.00 0.00 C ATOM 802 OE1 GLU A 57155.525 -11.806 8.817 1.00 0.00 O **ATOM** 803 OE2 GLU A 57157.435 -11.596 9.885 1.00 0.00 O ATOM

804 H GLUA 57154.880 -11.552 6.790 1.00 0.00 H 805 HA GLU A 57156.074 -9.242 5.579 1.00 0.00 H ATOM 806 1HB GLU A 57157.370 -11.760 6.641 1.00 0.00 H **ATOM** 807 2HB GLU A 57158.206 -10.268 6.231 1.00 0.00 H **ATOM** ATOM 808 1HG GLU A 57157.977 -9.732 8.374 1.00 0.00 H ATOM 809 2HG GLU A 57156.284 -9.419 7.995 1.00 0.00 H 810 N CYS A 58155.911 -10.214 3.224 1.00 0.00 N ATOM 811 CA CYS A 58156.129 -10.631 1.844 1.00 0.00 C **ATOM** 812 C CYS A 58157.505 -10.192 1.354 1.00 0.00 C ATOM 813 O CYS A 58157.859 -9.016 1.437 1.00 0.00 O **ATOM** 814 CB CYS A 58155.043 -10.051 0.935 1.00 0.00 C ATOM 815 SG CYS A 58153.516 -11.020 0.901 1.00 0.00 S ATOM 816 H CYS A 58155.341 -9.436 3.404 1.00 0.00 H ATOM 817 HA CYS A 58156.076 -11.709 1.812 1.00 0.00 H ATOM **ATOM** 818 1HB CYS A 58154.793 -9.057 1.275 1.00 0.00 H 819 2HB CYS A 58155,420 -9.996 -0.075 1.00 0.00 H **ATOM ATOM** 820 HG CYS A 58153.511 -11.593 1.672 1.00 0.00 H 821 N ALAA 59158.278 -11.145 0.842 1.00 0.00 N ATOM 822 CA ALA A 59159.615 -10.857 0.338 1.00 0.00 C **ATOM** 823 C ALA A 59159.552 -10.057 -0.958 1.00 0.00 C ATOM 824 O ALAA 59159.080 -10.551 -1.981 1.00 0.00 O **ATOM** 825 CB ALAA 59160.388 -12.149 0.126 1.00 0.00 C **ATOM** 826 H ALAA 59157.939 -12.064 0.802 1.00 0.00 H **ATOM** 827 HA ALA A 59160.133 -10.274 1.085 1.00 0.00 H **ATOM** 828 1HB ALA A 59159.764 -12.860 -0.395 1.00 0.00 H ATOM 829 2HB ALA A 59160.677 -12.557 1.084 1.00 0.00 H ATOM 830 3HB ALA A 59161.272 -11.948 -0.460 1.00 0.00 H ATOM 831 N GLYA 60160.031 -8.818 -0.907 1.00 0.00 N ATOM 832 CA GLY A 60160.020 -7.970 -2.084 1.00 0.00 C ATOM **ATOM** 833 C GLY A 60159.553 -6.560 -1.778 1.00 0.00 C ATOM 834 O GLY A 60159.945 -5.608 -2.455 1.00 0.00 O

- ATOM 835 H GLY A 60160.396 -8.478 -0.063 1.00 0.00 H
- ATOM 836 1HA GLY A 60161.020 -7.926 -2.491 1.00 0.00 H
- ATOM 837 2HA GLY A 60159.362 -8.403 -2.821 1.00 0.00 H
- ATOM 838 N CYS A 61158.713 -6.425 -0.757 1.00 0.00 N
- ATOM 839 CA CYS A 61158.192 -5.122 -0.363 1.00 0.00 C
- ATOM 840 C CYS A 61159.189 -4.380 0.519 1.00 0.00 C
- ATOM 841 O CYS A 61160.222 -4.931 0.904 1.00 0.00 O
- ATOM 842 CB CYS A 61156.861 -5.283 0.375 1.00 0.00 C
- ATOM 843 SG CYS A 61155.608 -6.197 -0.553 1.00 0.00 S
- ATOM 844 H CYS A 61158.438 -7.221 -0.257 1.00 0.00 H
- ATOM 845 HA CYS A 61158.026 -4.545 -1.262 1.00 0.00 H
- ATOM 846 1HB CYS A 61157.035 -5.812 1.301 1.00 0.00 H
- ATOM 847 2HB CYS A 61156.460 -4.305 0.595 1.00 0.00 H
- ATOM 848 HG CYS A 61154.811 -5.662 -0.582 1.00 0.00 H
- ATOM 849 N THR A 62158.876 -3.128 0.835 1.00 0.00 N
- ATOM 850 CA THR A 62159.746 -2.310 1.673 1.00 0.00 C
- ATOM 851 C THR A 62159.171 -2.169 3.078 1.00 0.00 C
- ATOM 852 O THR A 62158.132 -2.748 3.397 1.00 0.00 O
- ATOM 853 CB THR A 62159.940 -0.929 1.047 1.00 0.00 C
- ATOM 854 OG1 THR A 62158.694 -0.283 0.860 1.00 0.00 O
- ATOM 855 CG2 THR A 62160.641 -0.973 -0.294 1.00 0.00 C
- ATOM 856 H THR A 62158.040 -2.744 0.498 1.00 0.00 H
- ATOM 857 HA THR A 62160.704 -2.805 1.737 1.00 0.00 H
- ATOM 858 HB THR A 62160.540 -0.325 1.712 1.00 0.00 H
- ATOM 859 HG1 THR A 62158.840 0.602 0.518 1.00 0.00 H
- ATOM 860 1HG2 THR A 62160.440 -1.919 -0.774 1.00 0.00 H
- ATOM 861 2HG2 THR A 62161.705 -0.862 -0.148 1.00 0.00 H
- ATOM 862 3HG2 THR A 62160.277 -0.169 -0.917 1.00 0.00 H
- ATOM 863 N ASPA 63159.853 -1.394 3.916 1.00 0.00 N
- ATOM 864 CA ASP A 63159.410 -1.175 5.289 1.00 0.00 C
- ATOM 865 C ASPA 63158.661 0.148 5.414 1.00 0.00 C

866 O ASPA 63158.703 0.800 6.457 1.00 0.00 O **ATOM** 867 CB ASPA 63160.606 -1.189 6.241 1.00 0.00 C **ATOM** 868 CG ASPA 63161.704 -0.240 5.805 1.00 0.00 C **ATOM ATOM** 869 OD1 ASP A 63161.752 0.893 6.328 1.00 0.00 O 870 OD2 ASP A 63162.517 -0.629 4.939 1.00 0.00 O **ATOM ATOM** 871 H ASPA 63160.674 -0.958 3.604 1.00 0.00 H **ATOM** 872 HA ASPA 63158.741 -1.980 5.553 1.00 0.00 H 873 1HB ASPA 63160.276 -0.899 7.227 1.00 0.00 H **ATOM** 874 2HB ASPA 63161.013 -2.189 6.282 1.00 0.00 H **ATOM** 875 N GLYA 64157.976 0.538 4.344 1.00 0.00 N **ATOM** 876 CA GLY A 64157.227 1.781 4.356 1.00 0.00 C **ATOM** 877 C GLYA 64157,980 2.918 3.692 1.00 0.00 C ATOM **ATOM** 878 O GLY A 64158.006 4.037 4.204 1.00 0.00 O **ATOM** 879 H GLY A 64157.978 -0.022 3.540 1.00 0.00 H 880 1HA GLY A 64156.292 1.631 3.836 1.00 0.00 H **ATOM** 881 2HA GLY A 64157.018 2.053 5.380 1.00 0.00 H **ATOM** 882 N THR A 65158.594 2.630 2.549 1.00 0.00 N **ATOM** 883 CA THR A 65159.351 3.636 1.814 1.00 0.00 C ATOM 884 C THR A 65159.077 3.536 0.317 1.00 0.00 C **ATOM** 885 O THR A 65159.346 2.511 -0.307 1.00 0.00 O ATOM 886 CB THR A 65160.848 3.475 2.081 1.00 0.00 C **ATOM** 887 OG1 THR A 65161.266 2.148 1.810 1.00 0.00 O **ATOM** 888 CG2 THR A 65161.239 3.795 3.508 1.00 0.00 C **ATOM** 889 H THR A 65158.536 1.720 2.192 1.00 0.00 H **ATOM** 890 HA THR A 65159.035 4.608 2.162 1.00 0.00 H **ATOM** 891 HB THR A 65161.394 4.143 1.431 1.00 0.00 H **ATOM** 892 HG1 THR A 65161.056 1.927 0.900 1.00 0.00 H **ATOM** 893 1HG2 THR A 65160.578 4.555 3.900 1.00 0.00 H **ATOM** 894 2HG2 THR A 65162.256 4.158 3.530 1.00 0.00 H **ATOM** ATOM 895 3HG2 THR A 65161.162 2.904 4.112 1.00 0.00 H ATOM 896 N PHE A 66158.540 4.610 -0.254 1.00 0.00 N

897 CA PHE A 66158.230 4.645 -1.678 1.00 0.00 C ATOM 898 C PHE A 66159.285 5.435 -2.446 1.00 0.00 C **ATOM** 899 O PHE A 66159.348 6.660 -2.351 1.00 0.00 O **ATOM ATOM** 900 CB PHE A 66156.848 5.261 -1.905 1.00 0.00 C 901 CG PHE A 66156.258 4.935 -3.248 1.00 0.00 C ATOM 902 CD1 PHE A 66155.882 5.945 -4.118 1.00 0.00 C ATOM 903 CD2 PHE A 66156.081 3.618 -3.638 1.00 0.00 C ATOM 904 CE1 PHE A 66155.340 5.647 -5.354 1.00 0.00 C **ATOM** 905 CE2 PHE A 66155.538 3.314 -4.873 1.00 0.00 C **ATOM** 906 CZ PHE A 66155.167 4.330 -5.732 1.00 0.00 C **ATOM** 907 H PHE A 66158.348 5.398 0.296 1.00 0.00 H **ATOM** 908 HA PHE A 66158.224 3.628 -2.040 1.00 0.00 H **ATOM** 909 1HB PHE A 66156.171 4.898 -1.148 1.00 0.00 H **ATOM** 910 2HB PHE A 66156.925 6.337 -1.827 1.00 0.00 H ATOM 911 HD1 PHE A 66156.018 6.976 -3.824 1.00 0.00 H **ATOM** 912 HD2 PHE A 66156.370 2.822 -2.968 1.00 0.00 H ATOM 913 HE1 PHE A 66155.051 6.445 -6.023 1.00 0.00 H **ATOM ATOM** 914 HE2 PHE A 66155.404 2.283 -5.166 1.00 0.00 H 915 HZ PHE A 66154.743 4.096 -6.696 1.00 0.00 H **ATOM** 916 N ARGA 67160.111 4.724 -3.207 1.00 0.00 N **ATOM** 917 CA ARG A 67161.164 5.358 -3.991 1.00 0.00 C **ATOM** 918 C ARG A 67162.128 6.124 -3.090 1.00 0.00 C **ATOM** 919 O ARG A 67162.576 7.219 -3.430 1.00 0.00 O **ATOM** 920 CB ARG A 67160.557 6.304 -5.029 1.00 0.00 C **ATOM** 921 CG ARG A 67159.739 5.593 -6.096 1.00 0.00 C ATOM 922 CD ARG A 67160.131 6.041 -7.495 1.00 0.00 C **ATOM** 923 NE ARG A 67161.016 5.080 -8.150 1.00 0.00 N **ATOM** 924 CZ ARG A 67161.773 5.370 -9.206 1.00 0.00 C **ATOM** 925 NH1 ARG A 67161.755 6.590 -9.731 1.00 0.00 N **ATOM** 926 NH2 ARG A 67162.549 4.437 -9.741 1.00 0.00 N **ATOM** 927 H ARGA 67160.011 3.750 -3.241 1.00 0.00 H ATOM

ATOM 928 HA ARG A 67161.711 4.580 -4.503 1.00 0.00 H 929 1HB ARG A 67159.912 7.008 -4.523 1.00 0.00 H **ATOM** ATOM 930 2HB ARG A 67161.353 6.846 -5.516 1.00 0.00 H **ATOM** 931 1HG ARG A 67159.904 4.529 -6.012 1.00 0.00 H **ATOM** 932 2HG ARG A 67158.693 5.810 -5.938 1.00 0.00 H **ATOM** 933 1HD ARG A 67159.236 6.154 -8.088 1.00 0.00 H **ATOM** 934 2HD ARG A 67160.638 6.994 -7.425 1.00 0.00 H **ATOM** 935 HE ARG A 67161.048 4.172 -7.783 1.00 0.00 H **ATOM** 936 1HH1 ARG A 67161.172 7.297 -9.333 1.00 0.00 H **ATOM** 937 2HH1 ARG A 67162.325 6.801 -10.524 1.00 0.00 H 938 1HH2 ARG A 67162.566 3.516 -9.351 1.00 0.00 H ATOM ATOM 939 2HH2 ARG A 67163.117 4.653 -10.535 1.00 0.00 H **ATOM** 940 N GLY A 68162.443 5.540 -1.939 1.00 0.00 N ATOM 941 CA GLY A 68163.351 6.182 -1.006 1.00 0.00 C 942 C GLY A 68162.706 7.342 -0.275 1.00 0.00 C **ATOM** ATOM 943 O GLYA 68163.385 8.287 0.127 1.00 0.00 O 944 H GLY A 68162.055 4.667 -1.721 1.00 0.00 H ATOM 945 1HA GLY A 68163.679 5.452 -0.281 1.00 0.00 H ATOM **ATOM** 946 2HA GLY A 68164.210 6.546 -1.550 1.00 0.00 H **ATOM** 947 N THR A 69161.389 7.272 -0.102 1.00 0.00 N 948 CA THR A 69160.651 8.325 0.585 1.00 0.00 C ATOM 949 C THR A 69159.735 7.739 1.654 1.00 0.00 C **ATOM** 950 O THR A 69158.604 7.347 1.369 1.00 0.00 O **ATOM** 951 CB THR A 69159.829 9.137 -0.417 1.00 0.00 C **ATOM ATOM** 952 OG1 THR A 69160.590 9.421 -1.578 1.00 0.00 O 953 CG2 THR A 69159.336 10.454 0.141 1.00 0.00 C **ATOM** 954 H THR A 69160.902 6.493 -0.445 1.00 0.00 H ATOM 955 HA THR A 69161.368 8.976 1.061 1.00 0.00 H **ATOM** 956 HB THR A 69158.965 8.558 -0.711 1.00 0.00 H ATOM ATOM 957 HG1 THR A 69161.292 10.038 -1.358 1.00 0.00 H ATOM 958 1HG2 THR A 69159.985 11.252 -0.190 1.00 0.00 H

959 2HG2 THR A 69159.340 10.412 1.220 1.00 0.00 H **ATOM** 960 3HG2 THR A 69158.331 10.639 -0.208 1.00 0.00 H ATOM 961 N ARGA 70160.232 7.682 2.886 1.00 0.00 N ATOM ATOM 962 CA ARG A 70159.457 7.143 3.998 1.00 0.00 C 963 C ARG A 70158.310 8.077 4.365 1.00 0.00 C ATOM 964 O ARGA 70158.529 9.234 4.725 1.00 0.00 O ATOM 965 CB ARG A 70160.359 6.919 5.213 1.00 0.00 C ATOM 966 CG ARG A 70159.662 6.210 6.364 1.00 0.00 C **ATOM** 967 CD ARG A 70159.925 6.903 7.691 1.00 0.00 C ATOM 968 NE ARG A 70159.851 5.977 8.819 1.00 0.00 N **ATOM** 969 CZ ARG A 70160.254 6.275 10.051 1.00 0.00 C ATOM 970 NH1 ARG A 70160.761 7.472 10.320 1.00 0.00 N ATOM **ATOM** 971 NH2 ARG A 70160.151 5.374 11.018 1.00 0.00 N 972 H ARGA 70161.141 8.009 3.050 1.00 0.00 H ATOM 973 HA ARG A 70159.048 6.193 3.686 1.00 0.00 H **ATOM** 974 1HB ARG A 70161.208 6.324 4.913 1.00 0.00 H **ATOM** 975 2HB ARG A 70160.709 7.878 5.567 1.00 0.00 H ATOM 976 1HG ARG A 70158.599 6.203 6.178 1.00 0.00 H **ATOM** 977 2HG ARG A 70160.026 5.194 6.421 1.00 0.00 H ATOM 978 1HD ARG A 70160.912 7.343 7.663 1.00 0.00 H ATOM 979 2HD ARG A 70159.189 7.682 7.827 1.00 0.00 H **ATOM** 980 HE ARG A 70159.482 5.085 8.647 1.00 0.00 H **ATOM** 981 1HH1 ARG A 70160.841 8.157 9.595 1.00 0.00 H **ATOM ATOM** 982 2HH1 ARG A 70161.062 7.690 11.248 1.00 0.00 H 983 1HH2 ARG A 70159.771 4.470 10.820 1.00 0.00 H ATOM 984 2HH2 ARG A 70160.454 5.598 11.945 1.00 0.00 H **ATOM** 985 N TYR A 71157.086 7.567 4.275 1.00 0.00 N ATOM 986 CA TYR A 71155.903 8.356 4.599 1.00 0.00 C ATOM 987 C TYR A 71155.381 8.004 5.988 1.00 0.00 C **ATOM** 988 O TYR A 71154.877 8.865 6.710 1.00 0.00 O **ATOM** ATOM 989 CB TYR A 71154.808 8.125 3.556 1.00 0.00 C

ATOM 990 CG TYR A 71155.153 8.667 2.187 1.00 0.00 C 991 CD1 TYR A 71155.218 7.826 1.083 1.00 0.00 C ATOM 992 CD2 TYR A 71155.413 10.018 1.998 1.00 0.00 C **ATOM** 993 CE1 TYR A 71155.533 8.316 -0.170 1.00 0.00 C **ATOM** 994 CE2 TYR A 71155.727 10.517 0.748 1.00 0.00 C ATOM **ATOM** 995 CZ TYR A 71155.786 9.662 -0.332 1.00 0.00 C 996 OH TYR A 71156.099 10.155 -1.578 1.00 0.00 O ATOM 997 H TYR A 71156.976 6.638 3.983 1.00 0.00 H **ATOM** 998 HA TYR A 71156.187 9.397 4.587 1.00 0.00 H **ATOM** 999 1HB TYR A 71154.633 7.064 3.458 1.00 0.00 H ATOM 1000 2HB TYR A 71153.901 8.607 3.886 1.00 0.00 H ATOM 1001 HD1 TYR A 71155.019 6.773 1.213 1.00 0.00 H ATOM 1002 HD2 TYR A 71155.367 10.685 2.846 1.00 0.00 H ATOM 1003 HE1 TYR A 71155.578 7.646 -1.016 1.00 0.00 H ATOM 1004 HE2 TYR A 71155.926 11.571 0.622 1.00 0.00 H ATOM 1005 HH TYR A 71155.373 9.983 -2.182 1.00 0.00 H ATOM 1006 N PHE A 72155.504 6.733 6.357 1.00 0.00 N ATOM 1007 CA PHE A 72155.045 6.266 7.659 1.00 0.00 C ATOM 1008 C PHE A 72156.020 5.251 8.248 1.00 0.00 C ATOM 1009 O PHE A 72157.052 4.949 7.649 1.00 0.00 O ATOM 1010 CB PHE A 72153.653 5.642 7.538 1.00 0.00 C ATOM 1011 CG PHE A 72153.543 4.631 6.433 1.00 0.00 C ATOM 1012 CD1 PHE A 72153.294 5.033 5.130 1.00 0.00 C ATOM 1013 CD2 PHE A 72153.689 3.278 6.696 1.00 0.00 C ATOM 1014 CE1 PHE A 72153.193 4.104 4.111 1.00 0.00 C ATOM 1015 CE2 PHE A 72153.588 2.345 5.682 1.00 0.00 C ATOM 1016 CZ PHE A 72153.340 2.759 4.388 1.00 0.00 C ATOM 1017 H PHE A 72155.914 6.094 5.737 1.00 0.00 H ATOM 1018 HA PHE A 72154.990 7.120 8.317 1.00 0.00 H ATOM 1019 1HB PHE A 72153.406 5.147 8.465 1.00 0.00 H ATOM 1020 2HB PHE A 72152.931 6.422 7.349 1.00 0.00 H

ATOM 1021 HD1 PHE A 72153.179 6.084 4.913 1.00 0.00 H ATOM 1022 HD2 PHE A 72153.884 2.954 7.708 1.00 0.00 H ATOM 1023 HE1 PHE A 72152.997 4.431 3.101 1.00 0.00 H ATOM 1024 HE2 PHE A 72153.705 1.294 5.901 1.00 0.00 H ATOM 1025 HZ PHE A 72153.262 2.032 3.593 1.00 0.00 H ATOM 1026 N THR A 73155.687 4.731 9.424 1.00 0.00 N ATOM 1027 CA THR A 73156.534 3.750 10.094 1.00 0.00 C ATOM 1028 C THR A 73155.833 2.399 10.188 1.00 0.00 C ATOM 1029 O THR A 73154.813 2.263 10.862 1.00 0.00 O ATOM 1030 CB THR A 73156.909 4.241 11.493 1.00 0.00 C ATOM 1031 OG1 THR A 73157.700 3.278 12.167 1.00 0.00 O ATOM 1032 CG2 THR A 73155.709 4.539 12.365 1.00 0.00 C ATOM 1033 H THR A 73154.851 5.012 9.852 1.00 0.00 H ATOM 1034 HA THR A 73157.434 3.636 9.510 1.00 0.00 H ATOM 1035 HB THR A 73157.486 5.150 11.401 1.00 0.00 H ATOM 1036 HG1 THR A 73158.049 3.660 12.976 1.00 0.00 H ATOM 1037 1HG2 THR A 73155.202 3.617 12.608 1.00 0.00 H ATOM 1038 2HG2 THR A 73155.032 5.192 11.834 1.00 0.00 H ATOM 1039 3HG2 THR A 73156.035 5.021 13.274 1.00 0.00 H ATOM 1040 N CYS A 74156.388 1.402 9.505 1.00 0.00 N ATOM 1041 CA CYS A 74155.816 0.060 9.512 1.00 0.00 C ATOM 1042 C CYS A 74156.913 -0.999 9.554 1.00 0.00 C ATOM 1043 O CYS A 74158.096 -0.687 9.422 1.00 0.00 O ATOM 1044 CB CYS A 74154.939 -0.148 8.276 1.00 0.00 C ATOM 1045 SG CYS A 74153.237 0.427 8.475 1.00 0.00 S ATOM 1046 H CYS A 74157.201 1.572 8.985 1.00 0.00 H ATOM 1047 HA CYS A 74155.205 -0.035 10.396 1.00 0.00 H ATOM 1048 1HB CYS A 74155.370 0.387 7.443 1.00 0.00 H ATOM 1049 2HB CYS A 74154.905 -1.202 8.042 1.00 0.00 H ATOM 1050 HG CYS A 74152.753 0.204 7.676 1.00 0.00 H ATOM 1051 N ALA A 75156.512 -2.252 9.739 1.00 0.00 N

ATOM 1052 CA ALA A 75157.461 -3.357 9.799 1.00 0.00 C ATOM 1053 C ALAA 75158.197 -3.521 8.474 1.00 0.00 C ATOM 1054 O ALA A 75157.960 -2.774 7.524 1.00 0.00 O ATOM 1055 CB ALA A 75156.745 -4.647 10.170 1.00 0.00 C ATOM 1056 H ALAA 75155.554 -2.438 9.837 1.00 0.00 H ATOM 1057 HA ALA A 75158.180 -3.137 10.574 1.00 0.00 H ATOM 1058 1HB ALA A 75156.801 -4.796 11.238 1.00 0.00 H ATOM 1059 2HB ALA A 75157.215 -5.478 9.665 1.00 0.00 H ATOM 1060 3HB ALA A 75155.709 -4.583 9.869 1.00 0.00 H ATOM 1061 N LEUA 76159.091 -4.502 8.416 1.00 0.00 N ATOM 1062 CA LEU A 76159.862 -4.764 7.206 1.00 0.00 C ATOM 1063 C LEU A 76159.161 -5.793 6.326 1.00 0.00 C ATOM 1064 O LEUA 76158.560 -6.745 6.825 1.00 0.00 O ATOM 1065 CB LEU A 76161.265 -5.256 7.566 1.00 0.00 C ATOM 1066 CG LEU A 76162.272 -4.153 7.899 1.00 0.00 C ATOM 1067 CD1 LEU A 76163.265 -4.636 8.945 1.00 0.00 C ATOM 1068 CD2 LEU A 76162.999 -3.700 6.642 1.00 0.00 C ATOM 1069 H LEUA 76159.236 -5.064 9.206 1.00 0.00 H ATOM 1070 HA LEU A 76159.945 -3.836 6.659 1.00 0.00 H ATOM 1071 1HB LEU A 76161.185 -5.912 8.421 1.00 0.00 H ATOM 1072 2HB LEU A 76161.650 -5.823 6.733 1.00 0.00 H ATOM 1073 HG LEU A 76161.745 -3.304 8.307 1.00 0.00 H ATOM 1074 1HD1 LEU A 76164.124 -5.069 8.454 1.00 0.00 H ATOM 1075 2HD1 LEU A 76162.795 -5.380 9.572 1.00 0.00 H ATOM 1076 3HD1 LEU A 76163.582 -3.801 9.554 1.00 0.00 H ATOM 1077 1HD2 LEU A 76162.395 -3.926 5.775 1.00 0.00 H ATOM 1078 2HD2 LEU A 76163.945 -4.216 6.567 1.00 0.00 H ATOM 1079 3HD2 LEU A 76163.173 -2.636 6.690 1.00 0.00 H ATOM 1080 N LYS A 77159.241 -5.595 5.014 1.00 0.00 N ATOM 1081 CA LYS A 77158.615 -6.506 4.063 1.00 0.00 C ATOM 1082 C LYS A 77157.102 -6.545 4.261 1.00 0.00 C

ATOM 1083 O LYS A 77156.473 -7.591 4.107 1.00 0.00 O ATOM 1084 CB LYS A 77159.196 -7.914 4.213 1.00 0.00 C ATOM 1085 CG LYS A 77160.695 -7.980 3.971 1.00 0.00 C ATOM 1086 CD LYS A 77161.038 -7.712 2.515 1.00 0.00 C ATOM 1087 CE LYS A 77162.514 -7.398 2.339 1.00 0.00 C ATOM 1088 NZ LYS A 77163.360 -8.619 2.449 1.00 0.00 N ATOM 1089 H LYS A 77159.734 -4.817 4.677 1.00 0.00 H ATOM 1090 HA LYS A 77158.826 -6.143 3.069 1.00 0.00 H ATOM 1091 1HB LYS A 77158.998 -8.268 5.213 1.00 0.00 H ATOM 1092 2HB LYS A 77158.709 -8.569 3.505 1.00 0.00 H ATOM 1093 1HG LYS A 77161.183 -7.239 4.587 1.00 0.00 H ATOM 1094 2HG LYS A 77161.050 -8.965 4.240 1.00 0.00 H ATOM 1095 1HD LYS A 77160.794 -8.586 1.931 1.00 0.00 H ATOM 1096 2HD LYS A 77160.456 -6.871 2.167 1.00 0.00 H ATOM 1097 1HE LYS A 77162.662 -6.956 1.364 1.00 0.00 H ATOM 1098 2HE LYS A 77162.813 -6.693 3.101 1.00 0.00 H ATOM 1099 1HZ LYS A 77162.813 -9.459 2.167 1.00 0.00 H ATOM 1100 2HZ LYS A 77163.682 -8.743 3.430 1.00 0.00 H ATOM 1101 3HZ LYS A 77164.191 -8.536 1.831 1.00 0.00 H ATOM 1102 N LYS A 78156.526 -5.398 4.602 1.00 0.00 N ATOM 1103 CA LYS A 78155.087 -5.300 4.821 1.00 0.00 C ATOM 1104 C LYS A 78154.565 -3.928 4.407 1.00 0.00 C ATOM 1105 O LYS A 78153.672 -3.373 5.047 1.00 0.00 O ATOM 1106 CB LYS A 78154.754 -5.564 6.291 1.00 0.00 C ATOM 1107 CG LYS A 78155.276 -6.897 6.803 1.00 0.00 C ATOM 1108 CD LYS A 78155,037 -7.051 8.296 1.00 0.00 C ATOM 1109 CE LYS A 78153.738 -7.786 8.580 1.00 0.00 C ATOM 1110 NZ LYS A 78153.489 -7.930 10.040 1.00 0.00 N ATOM 1111 H LYS A 78157.081 -4.597 4.709 1.00 0.00 H ATOM 1112 HA LYS A 78154.609 -6.053 4.212 1.00 0.00 H ATOM 1113 1HB LYS A 78155.187 -4.778 6.892 1.00 0.00 H

ATOM 1114 2HB LYS A 78153.682 -5.551 6.413 1.00 0.00 H ATOM 1115 1HG LYS A 78154.768 -7.695 6.283 1.00 0.00 H ATOM 1116 2HG LYS A 78156.337 -6.956 6.609 1.00 0.00 H ATOM 1117 1HD LYS A 78155.857 -7.608 8.726 1.00 0.00 H ATOM 1118 2HD LYS A 78154.992 -6.070 8.746 1.00 0.00 H ATOM 1119 1HE LYS A 78152.923 -7.233 8.138 1.00 0.00 H ATOM 1120 2HE LYS A 78153.790 -8.768 8.132 1.00 0.00 H ATOM 1121 1HZ LYS A 78152.472 -7.847 10.240 1.00 0.00 H ATOM 1122 2HZ LYS A 78153.995 -7.189 10.566 1.00 0.00 H ATOM 1123 3HZ LYS A 78153.820 -8.860 10.369 1.00 0.00 H ATOM 1124 N ALAA 79155.130 -3.385 3.333 1.00 0.00 N ATOM 1125 CA ALAA 79154.722 -2.078 2.834 1.00 0.00 C ATOM 1126 C ALA A 79154.661 -2.066 1.311 1.00 0.00 C ATOM 1127 O ALA A 79155.692 -2.045 0.638 1.00 0.00 O ATOM 1128 CB ALA A 79155.673 -1.002 3.334 1.00 0.00 C ATOM 1129 H ALA A 79155.838 -3.876 2.865 1.00 0.00 H ATOM 1130 HA ALA A 79153.737 -1.864 3.225 1.00 0.00 H ATOM 1131 1HB ALAA 79156.179 -1.352 4.222 1.00 0.00 H ATOM 1132 2HB ALAA 79155.115 -0.107 3.567 1.00 0.00 H ATOM 1133 3HB ALAA 79156.402 -0.782 2.568 1.00 0.00 H ATOM 1134 N LEU A 80153.445 -2.077 0.772 1.00 0.00 N ATOM 1135 CA LEU A 80153.250 -2.068 -0.674 1.00 0.00 C ATOM 1136 C LEUA 80152.372 -0.893 -1.095 1.00 0.00 C ATOM 1137 O LEUA 80151.191 -0.835 -0.752 1.00 0.00 O ATOM 1138 CB LEU A 80152.617 -3.383 -1.131 1.00 0.00 C ATOM 1139 CG LEU A 80152.301 -3.464 -2.626 1.00 0.00 C ATOM 1140 CD1 LEU A 80153.582 -3.431 -3.445 1.00 0.00 C ATOM 1141 CD2 LEU A 80151.501 -4.721 -2.933 1.00 0.00 C ATOM 1142 H LEU A 80152.662 -2.093 1.360 1.00 0.00 H ATOM 1143 HA LEU A 80154.218 -1.962 -1.139 1.00 0.00 H ATOM 1144 1HB LEU A 80153.294 -4.189 -0.883 1.00 0.00 H

ATOM 1145 2HB LEU A 80151.698 -3.526 -0.585 1.00 0.00 H ATOM 1146 HG LEU A 80151.704 -2.608 -2.907 1.00 0.00 H ATOM 1147 1HD1 LEU A 80153.460 -4.038 -4.330 1.00 0.00 H ATOM 1148 2HD1 LEU A 80154.399 -3.819 -2.852 1.00 0.00 H ATOM 1149 3HD1 LEU A 80153.799 -2.413 -3.734 1.00 0.00 H ATOM 1150 1HD2 LEU A 80151.751 -5.074 -3.924 1.00 0.00 H ATOM 1151 2HD2 LEU A 80150.446 -4.496 -2.887 1.00 0.00 H ATOM 1152 3HD2 LEU A 80151.739 -5.485 -2.209 1.00 0.00 H ATOM 1153 N PHE A 81152.956 0.039 -1.839 1.00 0.00 N ATOM 1154 CA PHE A 81152.227 1.212 -2.307 1.00 0.00 C ATOM 1155 C PHE A 81151.468 0.904 -3.594 1.00 0.00 C ATOM 1156 O PHE A 81151.964 0.183 -4.460 1.00 0.00 O ATOM 1157 CB PHE A 81153.188 2.379 -2.536 1.00 0.00 C ATOM 1158 CG PHE A 81153.792 2.916 -1.270 1.00 0.00 C ATOM 1159 CD1 PHE A 81154.989 2.410 -0.788 1.00 0.00 C ATOM 1160 CD2 PHE A 81153.164 3.928 -0.561 1.00 0.00 C ATOM 1161 CE1 PHE A 81155.547 2.902 0.377 1.00 0.00 C ATOM 1162 CE2 PHE A 81153.717 4.425 0.603 1.00 0.00 C ATOM 1163 CZ PHE A 81154.910 3.911 1.073 1.00 0.00 C ATOM 1164 H PHE A 81153.900 -0.064 -2.079 1.00 0.00 H ATOM 1165 HA PHE A 81151.516 1.487 -1.543 1.00 0.00 H ATOM 1166 1HB PHE A 81153.995 2.052 -3.175 1.00 0.00 H ATOM 1167 2HB PHE A 81152.657 3.185 -3.020 1.00 0.00 H ATOM 1168 HD1 PHE A 81155.488 1.622 -1.332 1.00 0.00 H ATOM 1169 HD2 PHE A 81152.231 4.330 -0.928 1.00 0.00 H ATOM 1170 HE1 PHE A 81156.480 2.499 0.742 1.00 0.00 H ATOM 1171 HE2 PHE A 81153.216 5.213 1.146 1.00 0.00 H ATOM 1172 HZ PHE A 81155.344 4.297 1.983 1.00 0.00 H ATOM 1173 N VALA 82150.265 1.454 -3.713 1.00 0.00 N ATOM 1174 CA VALA 82149.439 1.238 -4.894 1.00 0.00 C ATOM 1175 C VALA 82148.475 2.400 -5.112 1.00 0.00 C

ATOM 1176 O VALA 82148.288 3.238 -4.230 1.00 0.00 O ATOM 1177 CB VALA 82148.632 -0.069 -4.784 1.00 0.00 C ATOM 1178 CG1 VAL A 82149.555 -1.276 -4.862 1.00 0.00 C ATOM 1179 CG2 VAL A 82147.821 -0.090 -3.498 1.00 0.00 C ATOM 1180 H VALA 82149.925 2.020 -2.988 1.00 0.00 H ATOM 1181 HA VALA 82150.095 1.161 -5.750 1.00 0.00 H ATOM 1182 HB VALA 82147.946 -0.116 -5.618 1.00 0.00 H ATOM 1183 1HG1 VAL A 82150.262 -1.240 -4.048 1.00 0.00 H ATOM 1184 2HG1 VAL A 82150.086 -1.262 -5.802 1.00 0.00 H ATOM 1185 3HG1 VAL A 82148.970 -2.181 -4.792 1.00 0.00 H ATOM 1186 1HG2 VAL A 82147.469 0.907 -3.279 1.00 0.00 H ATOM 1187 2HG2 VAL A 82148.442 -0.439 -2.686 1.00 0.00 H ATOM 1188 3HG2 VAL A 82146.976 -0.752 -3.616 1.00 0.00 H ATOM 1189 N LYS A 83147.867 2.443 -6.292 1.00 0.00 N ATOM 1190 CA LYS A 83146.922 3.502 -6.627 1.00 0.00 C ATOM 1191 C LYS A 83145.691 3.437 -5.732 1.00 0.00 C ATOM 1192 O LYS A 83145.092 2.376 -5.556 1.00 0.00 O ATOM 1193 CB LYS A 83146.505 3.398 -8.096 1.00 0.00 C ATOM 1194 CG LYS A 83147.637 3.674 -9.071 1.00 0.00 C ATOM 1195 CD LYS A 83147.323 3.133 -10.456 1.00 0.00 C ATOM 1196 CE LYS A 83148.071 3.897 -11.536 1.00 0.00 C ATOM 1197 NZ LYS A 83149.309 3.187 -11.962 1.00 0.00 N ATOM 1198 H LYS A 83148.058 1.747 -6.955 1.00 0.00 H ATOM 1199 HA LYS A 83147.415 4.449 -6.470 1.00 0.00 H ATOM 1200 1HB LYS A 83146.134 2.401 -8.281 1.00 0.00 H ATOM 1201 2HB LYS A 83145.714 4.108 -8.285 1.00 0.00 H ATOM 1202 1HG LYS A 83147.789 4.740 -9.138 1.00 0.00 H ATOM 1203 2HG LYS A 83148.538 3.203 -8.705 1.00 0.00 H ATOM 1204 1HD LYS A 83147.611 2.093 -10.500 1.00 0.00 H ATOM 1205 2HD LYS A. 83146.261 3.221 -10.634 1.00 0.00 H ATOM 1206 1HE LYS A 83147.422 4.015 -12.391 1.00 0.00 H

ATOM 1207 2HE LYS A 83148.339 4.871 -11.150 1.00 0.00 H ATOM 1208 1HZ LYS A 83149.120 2.620 -12.814 1.00 0.00 H ATOM 1209 2HZ LYS A 83149.638 2.556 -11.205 1.00 0.00 H ATOM 1210 3HZ LYS A 83150.060 3.875 -12.176 1.00 0.00 H ATOM 1211 N LEU A 84145.318 4.580 -5.169 1.00 0.00 N ATOM 1212 CA LEU A 84144.158 4.661 -4.291 1.00 0.00 C ATOM 1213 C LEU A 84142.865 4.491 -5.082 1.00 0.00 C ATOM 1214 O LEU A 84141.879 3.961 -4.572 1.00 0.00 O ATOM 1215 CB LEU A 84144.151 6.002 -3.554 1.00 0.00 C ATOM 1216 CG LEU A 84142.910 6.266 -2.698 1.00 0.00 C ATOM 1217 CD1 LEU A 84142.912 5.375 -1.467 1.00 0.00 C ATOM 1218 CD2 LEU A 84142.843 7.733 -2.298 1.00 0.00 C ATOM 1219 H LEU A 84145.837 5.392 -5.350 1.00 0.00 H ATOM 1220 HA LEU A 84144.233 3.863 -3.568 1.00 0.00 H ATOM 1221 1HB LEU A 84145.020 6.041 -2.914 1.00 0.00 H ATOM 1222 2HB LEU A 84144.229 6.791 -4.287 1.00 0.00 H ATOM 1223 HG LEU A 84142.027 6.036 -3.275 1.00 0.00 H ATOM 1224 1HD1 LEU A 84143.333 4.414 -1.719 1.00 0.00 H ATOM 1225 2HD1 LEU A 84141.899 5.244 -1.115 1.00 0.00 H ATOM 1226 3HD1 LEU A 84143.505 5.835 -0.689 1.00 0.00 H ATOM 1227 1HD2 LEU A 84142.606 8.332 -3.164 1.00 0.00 H ATOM 1228 2HD2 LEU A 84143.798 8.040 -1.898 1.00 0.00 H ATOM 1229 3HD2 LEU A 84142.078 7.866 -1.547 1.00 0.00 H ATOM 1230 N LYS A 85142.879 4.942 -6.332 1.00 0.00 N ATOM 1231 CA LYS A 85141.709 4.839 -7.195 1.00 0.00 C ATOM 1232 C LYS A 85141.357 3.378 -7.464 1.00 0.00 C ATOM 1233 O LYS A 85140.198 3.045 -7.713 1.00 0.00 O ATOM 1234 CB LYS A 85141.956 5.567 -8.517 1.00 0.00 C ATOM 1235 CG LYS A 85143.160 5.042 -9.284 1.00 0.00 C ATOM 1236 CD LYS A 85144.320 6.026 -9.247 1.00 0.00 C ATOM 1237 CE LYS A 85144.051 7.236 -10.128 1.00 0.00 C

ATOM 1238 NZ LYS A 85144.712 7.112 -11.457 1.00 0.00 N ATOM 1239 H LYS A 85143.696 5.354 -6.683 1.00 0.00 H ATOM 1240 HA LYS A 85140.880 5.308 -6.686 1.00 0.00 H ATOM 1241 1HB LYS A 85141.083 5.459 -9.143 1.00 0.00 H ATOM 1242 2HB LYS A 85142.114 6.616 -8.313 1.00 0.00 H ATOM 1243 1HG LYS A 85143.479 4.111 -8.842 1.00 0.00 H ATOM 1244 2HG LYS A 85142.875 4.876 -10.312 1.00 0.00 H ATOM 1245 1HD LYS A 85144.464 6.360 -8.231 1.00 0.00 H ATOM 1246 2HD LYS A 85145.212 5.528 -9.596 1.00 0.00 H ATOM 1247 1HE LYS A 85142.985 7.331 -10.273 1.00 0.00 H ATOM 1248 2HE LYS A 85144.426 8.119 -9.630 1.00 0.00 H ATOM 1249 1HZ LYS A 85145.717 6.869 -11.335 1.00 0.00 H ATOM 1250 2HZ LYS A 85144.645 8.011 -11.975 1.00 0.00 H ATOM 1251 3HZ LYS A 85144.251 6.367 -12.017 1.00 0.00 H ATOM 1252 N SER A 86142.363 2.511 -7.412 1.00 0.00 N ATOM 1253 CA SER A 86142.158 1.087 -7.651 1.00 0.00 C ATOM 1254 C SER A 86142.188 0.306 -6.341 1.00 0.00 C ATOM 1255 O SER A 86142.608 -0.850 -6.306 1.00 0.00 O ATOM 1256 CB SER A 86143.227 0.549 -8.603 1.00 0.00 C ATOM 1257 OG SER A 86143.165 1.200 -9.861 1.00 0.00 O ATOM 1258 H SER A 86143.265 2.837 -7.209 1.00 0.00 H ATOM 1259 HA SER A 86141.187 0.965 -8.107 1.00 0.00 H ATOM 1260 1HB SER A 86144.204 0.714 -8.176 1.00 0.00 H ATOM 1261 2HB SER A 86143.073 -0.510 -8.752 1.00 0.00 H ATOM 1262 HG SER A 86142.249 1.269 -10.141 1.00 0.00 H ATOM 1263 N CYS A 87141.740 0.946 -5.266 1.00 0.00 N ATOM 1264 CA CYS A 87141.714 0.312 -3.953 1.00 0.00 C ATOM 1265 C CYS A 87140.288 -0.056 -3.555 1.00 0.00 C ATOM 1266 O CYS A 87139.363 0.738 -3.721 1.00 0.00 O ATOM 1267 CB CYS A 87142.326 1.241 -2.903 1.00 0.00 C ATOM 1268 SG CYS A 87144.133 1.202 -2.848 1.00 0.00 S

ATOM 1269 H CYS A 87141.417 1.868 -5.358 1.00 0.00 H ATOM 1270 HA CYS A 87142.303 -0.591 -4.011 1.00 0.00 H ATOM 1271 1HB CYS A 87142.027 2.256 -3.113 1.00 0.00 H ATOM 1272 2HB CYS A 87141.961 0.958 -1.927 1.00 0.00 H ATOM 1273 HG CYS A 87144.438 0.603 -3.533 1.00 0.00 H ATOM 1274 N ARG A 88140.119 -1.265 -3.030 1.00 0.00 N ATOM 1275 CA ARG A 88138.806 -1.737 -2.610 1.00 0.00 C ATOM 1276 C ARG A 88138.683 -1.722 -1.085 1.00 0.00 C ATOM 1277 O ARG A 88139.522 -2.287 -0.385 1.00 0.00 O ATOM 1278 CB ARG A 88138.558 -3.152 -3.140 1.00 0.00 C ATOM 1279 CG ARG A 88137.514 -3.212 -4.244 1.00 0.00 C ATOM 1280 CD ARG A 88136.107 -3.286 -3.675 1.00 0.00 C ATOM 1281 NE ARGA 88135.160 -3.860 -4.628 1.00 0.00 N ATOM 1282 CZ ARG A 88133.845 -3.915 -4.425 1.00 0.00 C ATOM 1283 NH1 ARG A 88133.319 -3.434 -3.305 1.00 0.00 N ATOM 1284 NH2 ARG A 88133.055 -4.454 -5.343 1.00 0.00 N ATOM 1285 H ARG A 88140.895 -1.853 -2.924 1.00 0.00 H ATOM 1286 HA ARG A 88138.067 -1.072 -3.029 1.00 0.00 H ATOM 1287 1HB ARG A 88139.485 -3.544 -3.530 1.00 0.00 H ATOM 1288 2HB ARG A 88138.226 -3.779 -2.326 1.00 0.00 H ATOM 1289 1HG ARG A 88137.598 -2.327 -4.856 1.00 0.00 H ATOM 1290 2HG ARG A 88137.695 -4.089 -4.849 1.00 0.00 H ATOM 1291 1HD ARG A 88136.123 -3.898 -2.786 1.00 0.00 H ATOM 1292 2HD ARG A 88135.784 -2.288 -3.417 1.00 0.00 H ATOM 1293 HE ARG A 88135.522 -4.222 -5.463 1.00 0.00 H ATOM 1294 1HH1 ARG A 88133.909 -3.027 -2.609 1.00 0.00 H ATOM 1295 2HH1 ARG A 88132.330 -3.480 -3.158 1.00 0.00 H ATOM 1296 1HH2 ARG A 88133.446 -4.818 -6.189 1.00 0.00 H ATOM 1297 2HH2 ARG A 88132.067 -4.496 -5.191 1.00 0.00 H ATOM 1298 N PRO A 89137.633 -1.072 -0.548 1.00 0.00 N ATOM 1299 CA PRO A 89137.417 -0.994 0.901 1.00 0.00 C

ATOM 1300 C PRO A 89137.404 -2.369 1.559 1.00 0.00 C ATOM 1301 O PROA 89136.670 -3.264 1.136 1.00 0.00 O ATOM 1302 CB PRO A 89136.041 -0.332 1.024 1.00 0.00 C ATOM 1303 CG PRO A 89135.870 0.429 -0.245 1.00 0.00 C ATOM 1304 CD PRO A 89136.580 -0.368 -1.303 1.00 0.00 C ATOM 1305 HA PRO A 89138.161 -0.375 1.379 1.00 0.00 H ATOM 1306 1HB PRO A 89135.282 -1.091 1.136 1.00 0.00 H ATOM 1307 2HB PRO A 89136.031 0.326 1.881 1.00 0.00 H ATOM 1308 1HG PRO A 89134.819 0.515 -0.482 1.00 0.00 H ATOM 1309 2HG PRO A 89136.316 1.408 -0.150 1.00 0.00 H ATOM 1310 1HD PRO A 89135.902 -1.070 -1.765 1.00 0.00 H ATOM 1311 2HD PRO A 89137.011 0.289 -2.044 1.00 0.00 H ATOM 1312 N ASPA 90138.220 -2.533 2.594 1.00 0.00 N ATOM 1313 CA ASPA 90138.302 -3.801 3.309 1.00 0.00 C ATOM 1314 C ASP A 90137.533 -3.735 4.624 1.00 0.00 C ATOM 1315 O ASPA 90138.011 -3.166 5.606 1.00 0.00 O ATOM 1316 CB ASPA 90139.763 -4.165 3.578 1.00 0.00 C ATOM 1317 CG ASP A 90139.987 -5.664 3.624 1.00 0.00 C ATOM 1318 OD1 ASP A 90140.017 -6.226 4.739 1.00 0.00 O ATOM 1319 OD2 ASP A 90140.130 -6.275 2.544 1.00 0.00 O ATOM 1320 H ASPA 90138.781 -1.783 2.885 1.00 0.00 H ATOM 1321 HA ASP A 90137.860 -4.562 2.685 1.00 0.00 H ATOM 1322 1HB ASP A 90140.381 -3.751 2.796 1.00 0.00 H ATOM 1323 2HB ASP A 90140.063 -3.746 4.527 1.00 0.00 H ATOM 1324 N SER A 91136.339 -4.319 4.637 1.00 0.00 N ATOM 1325 CA SER A 91135.506 -4.326 5.834 1.00 0.00 C ATOM 1326 C SER A 91135.639 -5.649 6.582 1.00 0.00 C ATOM 1327 O SER A 91134.700 -6.099 7.237 1.00 0.00 O ATOM 1328 CB SER A 91134.042 -4.084 5.463 1.00 0.00 C ATOM 1329 OG SER A 91133.352 -3.424 6.510 1.00 0.00 O ATOM 1330 H SER A 91136.012 -4.757 3.824 1.00 0.00 H

ATOM 1331 HA SER A 91135.842 -3.527 6.476 1.00 0.00 H ATOM 1332 1HB SER A 91133.994 -3.472 4.575 1.00 0.00 H ATOM 1333 2HB SER A 91133.560 -5.032 5.272 1.00 0.00 H ATOM 1334 HG SER A 91133.254 -4.021 7.255 1.00 0.00 H ATOM 1335 N ARG A 92136.812 -6.266 6.479 1.00 0.00 N ATOM 1336 CA ARG A 92137.067 -7.537 7.147 1.00 0.00 C ATOM 1337 C ARG A 92137.066 -7.367 8.663 1.00 0.00 C ATOM 1338 O ARG A 92136.736 -8.295 9.401 1.00 0.00 O ATOM 1339 CB ARG A 92138.406 -8.118 6.689 1.00 0.00 C ATOM 1340 CG ARG A 92138.307 -8.944 5.417 1.00 0.00 C ATOM 1341 CD ARG A 92137.309 -10.081 5.568 1.00 0.00 C ATOM 1342 NE ARG A 92136.010 -9.750 4.987 1.00 0.00 N ATOM 1343 CZ ARG A 92134.911 -10.481 5.164 1.00 0.00 C ATOM 1344 NH1 ARG A 92134.949 -11.582 5.903 1.00 0.00 N ATOM 1345 NH2 ARG A 92133.771 -10.109 4.598 1.00 0.00 N ATOM 1346 H ARG A 92137.522 -5.857 5.942 1.00 0.00 H ATOM 1347 HA ARG A 92136.276 -8.219 6.873 1.00 0.00 H ATOM 1348 1HB ARG A 92139.095 -7.305 6.511 1.00 0.00 H ATOM 1349 2HB ARG A 92138.800 -8.748 7.472 1.00 0.00 H ATOM 1350 1HG ARGA 92137.988 -8.305 4.607 1.00 0.00 H ATOM 1351 2HG ARG A 92139.279 -9.357 5.191 1.00 0.00 H ATOM 1352 1HD ARG A 92137.701 -10.956 5.072 1.00 0.00 H ATOM 1353 2HD ARG A 92137.180 -10.293 6.619 1.00 0.00 H ATOM 1354 HE ARG A 92135.953 -8.941 4.437 1.00 0.00 H ATOM 1355 1HH1 ARG A 92135.807 -11.868 6.332 1.00 0.00 H ATOM 1356 2HH1 ARG A 92134.121 -12.127 6.032 1.00 0.00 H ATOM 1357 1HH2 ARG A 92133.736 -9.280 4.040 1.00 0.00 H ATOM 1358 2HH2 ARG A 92132.945 -10.658 4.730 1.00 0.00 H ATOM 1359 N PHE A 93137.439 -6.176 9.122 1.00 0.00 N ATOM 1360 CA PHE A 93137.481 -5.887 10.550 1.00 0.00 C ATOM 1361 C PHE A 93136.780 -4.569 10.863 1.00 0.00 C

ATOM 1362 O PHE A 93137.137 -3.875 11.815 1.00 0.00 O ATOM 1363 CB PHE A 93138.930 -5.835 11.037 1.00 0.00 C ATOM 1364 CG PHE A 93139.691 -7.106 10.797 1.00 0.00 C ATOM 1365 CD1 PHE A 93140.083 -7.907 11.858 1.00 0.00 C ATOM 1366 CD2 PHE A 93140.013 -7.503 9.508 1.00 0.00 C ATOM 1367 CE1 PHE A 93140.783 -9.078 11.639 1.00 0.00 C ATOM 1368 CE2 PHE A 93140.713 -8.673 9.283 1.00 0.00 C ATOM 1369 CZ PHE A 93141.098 -9.462 10.350 1.00 0.00 C ATOM 1370 H PHE A 93137.693 -5.476 8.484 1.00 0.00 H ATOM 1371 HA PHE A 93136.968 -6.685 11.065 1.00 0.00 H ATOM 1372 1HB PHE A 93139.446 -5.036 10.524 1.00 0.00 H ATOM 1373 2HB PHE A 93138.938 -5.637 12.100 1.00 0.00 H ATOM 1374 HD1 PHE A 93139.836 -7.607 12.866 1.00 0.00 H ATOM 1375 HD2 PHE A 93139.713 -6.887 8.674 1.00 0.00 H ATOM 1376 HE1 PHE A 93141.083 -9.693 12.475 1.00 0.00 H ATOM 1377 HE2 PHE A 93140.959 -8.971 8.275 1.00 0.00 H ATOM 1378 HZ PHE A 93141.645 -10.376 10.176 1.00 0.00 H ATOM 1379 N ALAA 94135.778 -4.230 10.057 1.00 0.00 N ATOM 1380 CA ALA A 94135.027 -2.996 10.252 1.00 0.00 C ATOM 1381 C ALA A 94133.691 -3.270 10.933 1.00 0.00 C ATOM 1382 O ALA A 94132.872 -4.038 10.431 1.00 0.00 O ATOM 1383 CB ALA A 94134.809 -2.296 8.918 1.00 0.00 C ATOM 1384 H ALAA 94135.538 -4.825 9.315 1.00 0.00 H ATOM 1385 HA ALA A 94135.614 -2.345 10.882 1.00 0.00 H ATOM 1386 1HB ALA A 94134.850 -3.021 8.120 1.00 0.00 H ATOM 1387 2HB ALA A 94135.580 -1.554 8.772 1.00 0.00 H ATOM 1388 3HB ALA A 94133.842 = 1.815 8.918 1.00 0.00 H ATOM 1389 N SER A 95133.478 -2.635 12.081 1.00 0.00 N ATOM 1390 CA SER A 95132.240 -2.810 12.832 1.00 0.00 C ATOM 1391 C SER A 95131.059 -2.200 12.085 1.00 0.00 C ATOM 1392 O SER A 95131.135 -1.074 11.594 1.00 0.00 O

ATOM 1393 CB SER A 95132.365 -2.173 14.217 1.00 0.00 C ATOM 1394 OG SER A 95131.405 -2.708 15.114 1.00 0.00 O ATOM 1395 H SER A 95134.169 -2.034 12.431 1.00 0.00 H ATOM 1396 HA SER A 95132.070 -3.870 12.947 1.00 0.00 H ATOM 1397 1HB SER A 95133.352 -2.365 14.611 1.00 0.00 H ATOM 1398 2HB SER A 95132.210 -1.108 14.137 1.00 0.00 H ATOM 1399 HG SER A 95130.544 -2.721 14.690 1.00 0.00 H ATOM 1400 N LEUA 96129.965 -2.952 12.003 1.00 0.00 N ATOM 1401 CA LEU A 96128.767 -2.486 11.316 1.00 0.00 C ATOM 1402 C LEU A 96127.508 -2.961 12.035 1.00 0.00 C ATOM 1403 O LEUA 96127.307 -4.159 12.230 1.00 0.00 O ATOM 1404 CB LEU A 96128.759 -2.981 9.868 1.00 0.00 C ATOM 1405 CG LEUA 96129.541 -2.112 8.882 1.00 0.00 C ATOM 1406 CD1 LEU A 96129.667 -2.811 7.537 1.00 0.00 C ATOM 1407 CD2 LEU A 96128.869 -0.757 8.719 1.00 0.00 C ATOM 1408 H LEUA 96129.965 -3.841 12.415 1.00 0.00 H ATOM 1409 HA LEU A 96128.783 -1.407 11.317 1.00 0.00 H ATOM 1410 1HB LEU A 96129.176 -3.978 9.849 1.00 0.00 H ATOM 1411 2HB LEU A 96127.733 -3.033 9.534 1.00 0.00 H ATOM 1412 HG LEU A 96130.537 -1.949 9.267 1.00 0.00 H ATOM 1413 1HD1 LEU A 96128.875 -2.478 6.882 1.00 0.00 H ATOM 1414 2HD1 LEU A 96129.590 -3.880 7.679 1.00 0.00 H ATOM 1415 3HD1 LEU A 96130.623 -2.574 7.096 1.00 0.00 H ATOM 1416 1HD2 LEU A 96128.830 -0.257 9.676 1.00 0.00 H ATOM 1417 2HD2 LEU A 96127.866 -0.895 8.344 1.00 0.00 H ATOM 1418 3HD2 LEU A 96129.435 -0.156 8.022 1.00 0.00 H ATOM 1419 N GLN A 97126.665 -2.011 12.428 1.00 0.00 N ATOM 1420 CA GLN A 97125.425 -2.332 13.127 1.00 0.00 C ATOM 1421 C GLN A 97124.243 -2.354 12.156 1.00 0.00 C ATOM 1422 O GLN A 97123.755 -1.304 11.739 1.00 0.00 O ATOM 1423 CB GLN A 97125.167 -1.315 14.240 1.00 0.00 C

ATOM 1424 CG GLN A 97125.424 -1.863 15.634 1.00 0.00 C ATOM 1425 CD GLN A 97124.146 -2.256 16.350 1.00 0.00 C ATOM 1426 OE1 GLN A 97123.962 -1.951 17.528 1.00 0.00 O ATOM 1427 NE2 GLN A 97123.255 -2.938 15.639 1.00 0.00 N ATOM 1428 H GLN A 97126.881 -1.073 12.244 1.00 0.00 H ATOM 1429 HA GLN A 97125.537 -3.311 13.565 1.00 0.00 H ATOM 1430 1HB GLN A 97125.810 -0.461 14.089 1.00 0.00 H ATOM 1431 2HB GLN A 97124.138 -0.993 14.187 1.00 0.00 H ATOM 1432 1HG GLN A 97126.055 -2.735 15.554 1.00 0.00 H ATOM 1433 2HG GLN A 97125.928 -1.107 16.218 1.00 0.00 H ATOM 1434 1HE2 GLN A 97123.470 -3.146 14.705 1.00 0.00 H ATOM 1435 2HE2 GLN A 97122.420 -3.205 16.076 1.00 0.00 H ATOM 1436 N PRO A 98123.766 -3.555 11.782 1.00 0.00 N ATOM 1437 CA PRO A 98122.638 -3.700 10.858 1.00 0.00 C ATOM 1438 C PRO A 98121.303 -3.372 11.518 1.00 0.00 C ATOM 1439 O PRO A 98121.041 -3.783 12.649 1.00 0.00 O ATOM 1440 CB PRO A 98122.694 -5.176 10.467 1.00 0.00 C ATOM 1441 CG PRO A 98123.315 -5.851 11.641 1.00 0.00 C ATOM 1442 CD PRO A 98124.286 -4.863 12.229 1.00 0.00 C ATOM 1443 HA PRO A 98122.765 -3.085 9.979 1.00 0.00 H ATOM 1444 1HB PRO A 98121.694 -5.541 10.282 1.00 0.00 H ATOM 1445 2HB PRO A 98123.298 -5.295 9.581 1.00 0.00 H ATOM 1446 1HG PRO A 98122.553 -6.103 12.364 1.00 0.00 H ATOM 1447 2HG PRO A 98123.834 -6.741 11.320 1.00 0.00 H ATOM 1448 1HD PRO A 98124.284 -4.928 13.307 1.00 0.00 H ATOM 1449 2HD PRO A 98125.279 -5.033 11.841 1.00 0.00 H ATOM 1450 N SER A 99120.462 -2.631 10.804 1.00 0.00 N ATOM 1451 CA SER A 99119.153 -2.249 11.322 1.00 0.00 C ATOM 1452 C SER A 99118.076 -3.219 10.847 1.00 0.00 C ATOM 1453 O SER A 99117.225 -3.649 11.627 1.00 0.00 O ATOM 1454 CB SER A 99118.803 -0.826 10.882 1.00 0.00 C

ATOM 1455 OG SER A 99117.906 -0.216 11.794 1.00 0.00 O ATOM 1456 H SER A 99120.727 -2.335 9,909 1.00 0.00 H ATOM 1457 HA SER A 99119.200 -2.282 12.399 1.00 0.00 H ATOM 1458 1HB SER A 99119.705 -0.235 10.834 1.00 0.00 H ATOM 1459 2HB SER A 99118.341 -0.857 9.907 1.00 0.00 H ATOM 1460 HG SER A 99117.119 0.070 11.326 1.00 0.00 H ATOM 1461 N GLY A 100118.117 -3.561 9.563 1.00 0.00 N ATOM 1462 CA GLY A 100117.140 -4.477 9.006 1.00 0.00 C ATOM 1463 C GLY A 100117.762 -5.478 8.050 1.00 0.00 C ATOM 1464 O GLY A 100118.930 -5.840 8.200 1.00 0.00 O ATOM 1465 H GLY A 100118.819 -3.187 8.988 1.00 0.00 H ATOM 1466 1HA GLY A 100116.667 -5.015 9.815 1.00 0.00 H ATOM 1467 2HA GLY A 100116.390 -3.909 8.478 1.00 0.00 H ATOM 1468 N PRO A 101117.001 -5.947 7.047 1.00 0.00 N ATOM 1469 CA PRO A 101117.498 -6.916 6.065 1.00 0.00 C ATOM 1470 C PRO A 101118.546 -6.311 5.135 1.00 0.00 C ATOM 1471 O PRO A 101119.493 -6.984 4.730 1.00 0.00 O ATOM 1472 CB PRO A 101116.244 -7.303 5.277 1.00 0.00 C ATOM 1473 CG PRO A 101115.329 -6.138 5.425 1.00 0.00 C ATOM 1474 CD PRO A 101115.598 -5.570 6.791 1.00 0.00 C ATOM 1475 HA PRO A 101117.909 -7.791 6.546 1.00 0.00 H ATOM 1476 1HB PRO A 101116.503 -7.474 4.243 1.00 0.00 H ATOM 1477 2HB PRO A 101115.813 -8.199 5.699 1.00 0.00 H ATOM 1478 1HG PRO A 101115.545 -5.402 4.664 1.00 0.00 H ATOM 1479 2HG PRO A 101114.302 -6.465 5.351 1.00 0.00 H ATOM 1480 1HD PRO A 101115.482 -4.497 6.784 1.00 0.00 H ATOM 1481 2HD PRO A 101114.940 -6.018 7.522 1.00 0.00 H ATOM 1482 N SER A 102118.367 -5.037 4.801 1.00 0.00 N ATOM 1483 CA SER A 102119.297 -4.341 3.919 1.00 0.00 C ATOM 1484 C SER A 102118.912 -2.873 3.773 1.00 0.00 C ATOM 1485 O SER A 102119.748 -1.983 3.931 1.00 0.00 O

ATOM 1486 CB SER A 102119.328 -5.012 2.544 1.00 0.00 C ATOM 1487 OG SER A 102118.028 -5.404 2.138 1.00 0.00 O ATOM 1488 H SER A 102117.592 -4.554 5.156 1.00 0.00 H ATOM 1489 HA SER A 102120.281 -4.401 4.361 1.00 0.00 H ATOM 1490 1HB SER A 102119.724 -4.319 1.817 1.00 0.00 H ATOM 1491 2HB SER A 102119.958 -5.888 2.587 1.00 0.00 H ATOM 1492 HG SER A 102117.584 -4.662 1.720 1.00 0.00 H ATOM 1493 N SER A 103117.641 -2.626 3.472 1.00 0.00 N ATOM 1494 CA SER A 103117.145 -1.265 3.305 1.00 0.00 C ATOM 1495 C SER A 103115.622 -1.246 3.240 1.00 0.00 C ATOM 1496 O SER A 103114.978 -2.295 3.195 1.00 0.00 O ATOM 1497 CB SER A 103117.729 -0.639 2.037 1.00 0.00 C ATOM 1498 OG SER A 103118.925 0.066 2.321 1.00 0.00 O ATOM 1499 H SER A 103117.022 -3.378 3.359 1.00 0.00 H ATOM 1500 HA SER A 103117.465 -0.689 4.160 1.00 0.00 H ATOM 1501 1HB SER A 103117.946 -1.417 1.321 1.00 0.00 H ATOM 1502 2HB SER A 103117.011 0.048 1.615 1.00 0.00 H ATOM 1503 HG SER A 103119.621 -0.234 1.732 1.00 0.00 H ATOM 1504 N GLY A 104115.049 -0.046 3.236 1.00 0.00 N ATOM 1505 CA GLY A 104113.605 0.086 3.176 1.00 0.00 C ATOM 1506 C GLY A 104113.168 1.467 2.728 1.00 0.00 C ATOM 1507 O GLY A 104112.708 2.251 3.585 1.00 0.00 O ATOM 1508 OXT GLY A 104113.285 1.764 1.521 1.00 0.00 O ATOM 1509 H GLY A 104115.612 0.755 3.273 1.00 0.00 H ATOM 1510 1HA GLY A 104113.216 -0.645 2.484 1.00 0.00 H ATOM 1511 2HA GLY A 104113.196 -0.108 4.157 1.00 0.00 H TER 1512 GLY A 104 **ENDMDL**

Three-Dimensional Structure Coordinate Table 9
ATOM 1 N GLY A 1127.996 -5.495 4.967 1.00 0.00 N

ATOM 2 CA GLY A 1127.436 -4.222 5.499 1.00 0.00 C ATOM 3 C GLY A 1127.407 -3.121 4.459 1.00 0.00 C ATOM 4 O GLY A 1126.530 -2.258 4.483 1.00 0.00 O ATOM 5 1H GLY A 1129.036 -5.459 4.975 1.00 0.00 H ATOM 6 2H GLY A 1127.674 -5.646 3.989 1.00 0.00 H ATOM 7 3H GLY A 1127.683 -6.296 5.551 1.00 0.00 H ATOM 8 1HA GLY A 1126.428 -4.402 5.845 1.00 0.00 H ATOM 9 2HA GLY A 1128.040 -3.898 6.334 1.00 0.00 H ATOM10 N SER A 2128.369 -3.150 3.543 1.00 0.00 N ATOM11 CA SER A 2128.452 -2.145 2.488 1.00 0.00 C ATOM12 C SER A 2127.262 -2.254 1.539 1.00 0.00 C ATOM13 O SER A 2126.460 -1.327 1.425 1.00 0.00 O ATOM14 CB SER A 2129.758 -2.301 1.707 1.00 0.00 C ATOM15 OG SER A 2130.194 -3.649 1.704 1.00 0.00 O ATOM16 H SER A 2129.040 -3.863 3.576 1.00 0.00 H ATOM17 HA SER A 2128.436 -1.172 2.956 1.00 0.00 H ATOM18 1HB SER A 2129.604 -1.984 0.686 1.00 0.00 H ATOM19 2HB SER A 2130.522 -1.688 2.163 1.00 0.00 H ATOM20 HG SER A 2130.040 -4.034 0.839 1.00 0.00 H ATOM21 N SER A 3127.155 -3.392 0.861 1.00 0.00 N ATOM22 CA SER A 3126.063 -3.622 -0.079 1.00 0.00 C ATOM23 C SER A 3124.712 -3.534 0.624 1.00 0.00 C ATOM24 O SER A 3124.618 -3.732 1.836 1.00 0.00 O ATOM25 CB SER A 3126.216 -4.989 -0.747 1.00 0.00 C ATOM26 OG SER A 3126.958 -4.889 -1.950 1.00 0.00 O ATOM27 H SER A 3127.825 -4.094 0.995 1.00 0.00 H ATOM28 HA SER A 3126.111 -2.853 -0.836 1.00 0.00 H ATOM29 1HB SER A 3126.733 -5.659 -0.076 1.00 0.00 H ATOM30 2HB SER A 3125.239 -5.388 -0.972 1.00 0.00 H ATOM31 HG SER A 3127.724 -4.327 -1.809 1.00 0.00 H ATOM32 N GLYA 4123.668 -3.236 -0.143 1.00 0.00 N

ATOM33 CA GLY A 4122.338 -3.127 0.425 1.00 0.00 C ATOM34 C GLY A 4122.252 -2.063 1.500 1.00 0.00 C ATOM35 O GLY A 4123.271 -1.522 1.928 1.00 0.00 O ATOM36 H GLY A 4123.804 -3.088 -1.103 1.00 0.00 H ATOM37 1HA GLY A 4121.641 -2.885 -0.364 1.00 0.00 H ATOM38 2HA GLY A 4122.062 -4.080 0.853 1.00 0.00 H ATOM39 N SER A 5121.032 -1.761 1.938 1.00 0.00 N ATOM40 CA SER A 5120.812 -0.752 2.971 1.00 0.00 C ATOM41 C SER A 5121.111 0.647 2.440 1.00 0.00 C ATOM42 O SER A 5120.218 1.488 2.344 1.00 0.00 O ATOM43 CB SER A 5121.680 -1.042 4.198 1.00 0.00 C ATOM44 OG SER A 5120.979 -0.763 5.397 1.00 0.00 O ATOM45 H SER A 5120.260 -2.229 1.555 1.00 0.00 H ATOM46 HA SER A 5119.773 -0.799 3.259 1.00 0.00 H ATOM47 1HB SER A 5121.964 -2.085 4.197 1.00 0.00 H ATOM48 2HB SER A 5122.568 -0.428 4.162 1.00 0.00 H ATOM49 HG SER A 5120.189 -1.306 5.440 1.00 0.00 H ATOM50 N SER A 6122.373 0.889 2.097 1.00 0.00 N ATOM51 CA SER A 6122.793 2.186 1.576 1.00 0.00 C ATOM52 C SER A 6122.700 3.261 2.653 1.00 0.00 C ATOM53 O SER A 6121.654 3.883 2.837 1.00 0.00 O ATOM54 CB SER A 6121.937 2.580 0.369 1.00 0.00 C ATOM55 OG SER A 6121.576 1.443 -0.394 1.00 0.00 O ATOM56 H SER A 6123.040 0.178 2.198 1.00 0.00 H ATOM57 HA SER A 6123.822 2.098 1.262 1.00 0.00 H ATOM58 1HB SER A 6121.038 3.068 0.713 1.00 0.00 H ATOM59 2HB SER A 6122.497 3.259 -0.259 1.00 0.00 H ATOM60 HG SER A 6120.764 1.623 -0.873 1.00 0.00 H ATOM61 N GLY A 7123.804 3.476 3.363 1.00 0.00 N ATOM62 CA GLY A 7123.829 4.477 4.412 1.00 0.00 C ATOM63 C GLY A 7125.104 5.296 4.400 1.00 0.00 C

ATOM64 O GLY A 7125.065 6.520 4.527 1.00 0.00 O ATOM65 H GLY A 7124.609 2.950 3.170 1.00 0.00 H ATOM66 1HA GLY A 7122.986 5.140 4.283 1.00 0.00 H ATOM67 2HA GLY A 7123.740 3.983 5.369 1.00 0.00 H ATOM68 N LEUA 8126.238 4.620 4.248 1.00 0.00 N ATOM69 CA LEU A 8127.532 5.292 4.219 1.00 0.00 C ATOM70 C LEUA 8128.105 5.309 2.805 1.00 0.00 C ATOM71_O LEUA 8128.927 4.466 2.448 1.00 0.00 O ATOM72 CB LEU A 8128.512 4.600 5.169 1.00 0.00 C ATOM73 CG LEU A 8127.931 4.217 6.531 1.00 0.00 C ATOM74 CD1 LEU A 8128.639 2.991 7.087 1.00 0.00 C ATOM75 CD2 LEU A 8128.039 5.384 7.502 1.00 0.00 C ATOM76 H LEUA 8126.204 3.645 4.152 1.00 0.00 H ATOM77 HA LEUA 8127.384 6.310 4.548 1.00 0.00 H ATOM78 1HB LEU A 8128.872 3.702 4.689 1.00 0.00 H ATOM79 2HB LEU A 8129.349 5.261 5.333 1.00 0.00 H ATOM80 HG LEU A 8126.885 3.974 6.415 1.00 0.00 H ATOM81 1HD1 LEU A 8128.427 2.901 8.143 1.00 0.00 H ATOM82 2HD1 LEU A 8129.705 3.094 6.942 1.00 0.00 H ATOM83 3HD1 LEU A 8128.288 2.108 6.573 1.00 0.00 H ATOM84 1HD2 LEU A 8127.268 5.299 8.253 1.00 0.00 H ATOM85 2HD2 LEU A 8127.917 6.312 6.964 1.00 0.00 H ATOM86 3HD2 LEU A 8129.008 5.368 7.978 1.00 0.00 H ATOM87 N ALAA 9127.663 6.274 2.004 1.00 0.00 N ATOM88 CA ALAA 9128.131 6.400 0.630 1.00 0.00 C ATOM89 C ALAA 9128.306 7.864 0.241 1.00 0.00 C ATOM90 O ALAA 9127.411 8.683 0.450 1.00 0.00 O ATOM91 CB ALA A 9127.166 5.710 -0.321 1.00 0.00 C ATOM92 H ALAA 9127.007 6.917 2.347 1.00 0.00 H ATOM93 HA ALA A 9129.088 5.903 0.558 1.00 0.00 H ATOM94 1HB ALA A 9126.500 6.444 -0.753 1.00 0.00 H

ATOM95 2HB ALA A 9126.588 4.976 0.222 1.00 0.00 H ATOM96 3HB ALA A 9127.721 5.222 -1.107 1.00 0.00 H ATOM97 N MET A 10129.464 8.186 -0.326 1.00 0.00 N ATOM98 CA MET A 10129.755 9.553 -0.746 1.00 0.00 C ATOM99 C MET A 10130.359 9.575 -2.148 1.00 0.00 C 100 O META 10131.577 9.500 -2.309 1.00 0.00 O ATOM 101 CB MET A 10130.713 10.218 0.244 1.00 0.00 C ATOM 102 CG META 10130.546 11.726 0.332 1.00 0.00 C ATOM 103 SD META 10132.032 12.556 0.926 1.00 0.00 S **ATOM** 104 CE META 10132.482 11.502 2.302 1.00 0.00 C ATOM ATOM 105 H META 10130.137 7.489 -0.466 1.00 0.00 H ATOM 106 HA META 10128.826 10.101 -0.756 1.00 0.00 H 107 1HB META 10130.546 9.801 1.225 1.00 0.00 H ATOM **ATOM** 108 2HB META 10131.728 10.008 -0.059 1.00 0.00 H 109 1HG META 10130.307 12.107 -0.649 1.00 0.00 H ATOM 110 2HG MET A 10129.733 11.945 1.009 1.00 0.00 H ATOM 111 1HE MET A 10131.660 10.838 2.531 1.00 0.00 H ATOM **ATOM** 112 2HE MET A 10132.704 12.111 3.166 1.00 0.00 H 113 3HE MET A 10133.353 10.919 2.040 1.00 0.00 H ATOM 114 N PROA 11129.510 9.679 -3.186 1.00 0.00 N ATOM 115 CA PRO A 11129.968 9.712 -4.578 1.00 0.00 C ATOM 116 C PROA 11130.980 10.829 -4.830 1.00 0.00 C ATOM 117 O PRO A 11132.013 10.604 -5.461 1.00 0.00 O ATOM 118 CB PRO A 11128.690 9.958 -5.383 1.00 0.00 C **ATOM** 119 CG PRO A 11127.575 9.536 -4.490 1.00 0.00 C ATOM 120 CD PRO A 11128.044 9.776 -3.082 1.00 0.00 C ATOM **ATOM** 121 HA PRO A 11130.404 8.768 -4.869 1.00 0.00 H 122 1HB PRO A 11128.619 11.004 -5.640 1.00 0.00 H **ATOM** 123 2HB PRO A 11128.714 9.365 -6.286 1.00 0.00 H **ATOM** 124 1HG PRO A 11126.699 10.131 -4.695 1.00 0.00 H ATOM 125 2HG PRO A 11127.361 8.488 -4.639 1.00 0.00 H

ATOM 126 1HD PRO A 11127.745 10.759 -2.747 1.00 0.00 H **ATOM** 127 2HD PRO A 11127.654 9.016 -2.420 1.00 0.00 H **ATOM** 128 N PRO A 12130.705 12.051 -4.336 1.00 0.00 N 129 CA PRO A 12131.611 13.191 -4.516 1.00 0.00 C **ATOM** 130 C PROA 12132.995 12.918 -3.938 1.00 0.00 C **ATOM** ATOM 131 O PROA 12133.971 13.573 -4.303 1.00 0.00 O **ATOM** 132 CB PRO A 12130.928 14.329 -3.749 1.00 0.00 C 133 CG PRO A 12129.499 13.920 -3.643 1.00 0.00 C ATOM 134 CD PRO A 12129.506 12.421 -3.563 1.00 0.00 C **ATOM ATOM** 135 HA PRO A 12131.705 13.460 -5.558 1.00 0.00 H ATOM 136 1HB PRO A 12131.382 14.431 -2.775 1.00 0.00 H **ATOM** 137 2HB PRO A 12131.033 15.251 -4.300 1.00 0.00 H **ATOM** 138 1HG PRO A 12129.061 14.342 -2.750 1.00 0.00 H **ATOM** 139 2HG PRO A 12128.957 14.246 -4.519 1.00 0.00 H **ATOM** 140 1HD PRO A 12129.593 12.098 -2.536 1.00 0.00 H 141 2HD PRO A 12128.615 12.015 -4.013 1.00 0.00 H **ATOM** 142 N GLY A 13133.070 11.946 -3.033 1.00 0.00 N ATOM 143 CA GLY A 13134.339 11.603 -2.418 1.00 0.00 C **ATOM** ATOM 144 C GLY A 13135.224 10.780 -3.333 1.00 0.00 C 145 O GLY A 13135.246 10.995 -4.545 1.00 0.00 O **ATOM** 146 H GLY A 13132.258 11.458 -2.781 1.00 0.00 H **ATOM ATOM** 147 1HA GLY A 13134.858 12.515 -2.158 1.00 0.00 H **ATOM** 148 2HA GLY A 13134.149 11.040 -1.517 1.00 0.00 H 149 N ASNA 14135.956 9.835 -2.753 1.00 0.00 N ATOM 150 CA ASN A 14136.846 8.976 -3.524 1.00 0.00 C ATOM 151 C ASN A 14136.100 7.759 -4.061 1.00 0.00 C **ATOM** 152 O ASN A 14136.231 7.404 -5.232 1.00 0.00 O **ATOM** 153 CB ASN A 14138.027 8.525 -2.662 1.00 0.00 C **ATOM** 154 CG ASN A 14138.857 9.692 -2.162 1.00 0.00 C **ATOM** 155 OD1 ASN A 14138.854 10.769 -2.756 1.00 0.00 O ATOM 156 ND2 ASN A 14139.573 9.481 -1.064 1.00 0.00 N ATOM

ATOM 157 H ASN A 14135.895 9.712 -1.782 1.00 0.00 H **ATOM** 158 HA ASN A 14137.220 9.551 -4.358 1.00 0.00 H **ATOM** 159 1HB ASN A 14137.653 7.982 -1.806 1.00 0.00 H 160 2HB ASN A 14138.663 7.876 -3.245 1.00 0.00 H **ATOM** 161 1HD2 ASN A 14139.527 8.597 -0.644 1.00 0.00 H **ATOM** 162 2HD2 ASN A 14140.120 10.217 -0.719 1.00 0.00 H **ATOM ATOM** 163 N SER A 15135.315 7.125 -3.196 1.00 0.00 N 164 CA SER A 15134.547 5.947 -3.583 1.00 0.00 C **ATOM** 165 C SER A 15133.644 5.488 -2.442 1.00 0.00 C **ATOM ATOM** 166 O SER A 15132.494 5.108 -2.662 1.00 0.00 O 167 CB SER A 15135.486 4.812 -3.996 1.00 0.00 C ATOM **ATOM** 168 OG SER A 15136.245 4.351 -2.892 1.00 0.00 O 169 H SER A 15135.251 7.455 -2.275 1.00 0.00 H **ATOM** 170 HA SER A 15133.930 6.217 -4.427 1.00 0.00 H **ATOM** 171 1HB SER A 15134.904 3.989 -4.385 1.00 0.00 H **ATOM** 172 2HB SER A 15136.162 5.168 -4.759 1.00 0.00 H **ATOM** 173 HG SER A 15137.023 4.903 -2.786 1.00 0.00 H ATOM 174 N HIS A 16134.175 5.525 -1.224 1.00 0.00 N **ATOM ATOM** 175 CA HIS A 16133.417 5.111 -0.049 1.00 0.00 C 176 C HIS A 16133.979 5.757 1.214 1.00 0.00 C **ATOM** 177 O HIS A 16133.236 6.307 2.026 1.00 0.00 O **ATOM** 178 CB HIS A 16133.435 3.586 0.086 1.00 0.00 C **ATOM** 179 CG HIS A 16132.079 2.962 -0.010 1.00 0.00 C ATOM 180 ND1 HIS A 16131.135 3.053 0.991 1.00 0.00 N ATOM 181 CD2 HIS A 16131.507 2.232 -0.998 1.00 0.00 C **ATOM** 182 CE1 HIS A 16130.042 2.407 0.624 1.00 0.00 C ATOM 183 NE2 HIS A 16130.242 1.900 -0.578 1.00 0.00 N **ATOM** 184 H HIS A 16135.097 5.836 -1.113 1.00 0.00 H ATOM 185 HA HIS A 16132.397 5.439 -0.181 1.00 0.00 H ATOM 186 1HB HIS A 16134.049 3.170 -0.699 1.00 0.00 H ATOM

187 2HB HIS A 16133.858 3.320 1.044 1.00 0.00 H

ATOM

188 HD1 HIS A 16131.249 3.521 1.845 1.00 0.00 H ATOM **ATOM** 189 HD2 HIS A 16131.962 1.962 -1.940 1.00 0.00 H ATOM 190 HE1 HIS A 16129.139 2.311 1.208 1.00 0.00 H ATOM 191 HE2 HIS A 16129.625 1.303 -1.049 1.00 0.00 H ATOM 192 N GLY A 17135.297 5.683 1.373 1.00 0.00 N ATOM 193 CA GLY A 17135.936 6.264 2.539 1.00 0.00 C 194 C GLY A 17137.228 5.562 2.903 1.00 0.00 C **ATOM** ATOM 195 O GLY A 17137.354 5.004 3.994 1.00 0.00 O 196 H GLY A 17135.839 5.232 0.693 1.00 0.00 H **ATOM** 197 1HA GLY A 17136.149 7.304 2.339 1.00 0.00 H ·ATOM 198 2HA GLY A 17135.257 6.203 3.377 1.00 0.00 H **ATOM** 199 N LEUA 18138.193 5.587 1.989 1.00 0.00 N **ATOM** ATOM 200 CA LEU A 18139.483 4.948 2.219 1.00 0.00 C 201 C LEUA 18140.546 5.982 2.577 1.00 0.00 C ATOM 202 O LEUA 18140.944 6.792 1.741 1.00 0.00 O ATOM ATOM 203 CB LEU A 18139.915 4.162 0.980 1.00 0.00 C 204 CG LEUA 18138.847 3.235 0.396 1.00 0.00 C ATOM 205 CD1 LEU A 18139.067 3.043 -1.097 1.00 0.00 C ATOM ATOM 206 CD2 LEU A 18138.857 1.894 1.114 1.00 0.00 C 207 H LEUA 18138.033 6.049 1.139 1.00 0.00 H ATOM 208 HA LEUA 18139.370 4.264 3.047 1.00 0.00 H ATOM 209 1HB LEUA 18140.207 4.868 0.216 1.00 0.00 H ATOM 210 2HB LEU A 18140.775 3.563 1.240 1.00 0.00 H ATOM ATOM 211 HG LEU A 18137.875 3.684 0.534 1.00 0.00 H ATOM 212 1HD1 LEU A 18138.111 2.991 -1.597 1.00 0.00 H 213 2HD1 LEU A 18139.612 2.126 -1.266 1.00 0.00 H ATOM 214 3HD1 LEU A 18139.632 3.876 -1.488 1.00 0.00 H **ATOM** 215 1HD2 LEU A 18137.880 1.440 1.041 1.00 0.00 H ATOM ATOM 216 2HD2 LEU A 18139.107 2.045 2.154 1.00 0.00 H ATOM 217 3HD2 LEU A 18139.590 1.246 0.658 1.00 0.00 H ATOM 218 N GLUA 19141.003 5.945 3.825 1.00 0.00 N

219 CA GLUA 19142.020 6.879 4.293 1.00 0.00 C ATOM 220 C GLUA 19143.006 6.186 5.228 1.00 0.00 C ATOM ATOM 221 O GLUA 19142.874 4.996 5.513 1.00 0.00 O ATOM 222 CB GLU A 19141.365 8.062 5.010 1.00 0.00 C 223 CG GLU A 19140.356 7.647 6.069 1.00 0.00 C **ATOM ATOM** 224 CD GLU A 19140.441 8.499 7.320 1.00 0.00 C ATOM 225 OE1 GLU A 19139.379 8.824 7.891 1.00 0.00 O 226 OE2 GLU A 19141.570 8.843 7.730 1.00 0.00 O **ATOM** 227 H GLUA 19140.647 5.276 4.445 1.00 0.00 H **ATOM ATOM** 228 HA GLUA 19142.556 7.246 3.431 1.00 0.00 H **ATOM** 229 1HB GLU A 19142.135 8.649 5.487 1.00 0.00 H ATOM 230 2HB GLU A 19140.856 8.674 4.280 1.00 0.00 H **ATOM** 231 1HG GLU A 19139.363 7.738 5.657 1.00 0.00 H **ATOM** 232 2HG GLUA 19140.540 6.618 6.340 1.00 0.00 H 233 N VALA 20143.994 6.939 5.702 1.00 0.00 N **ATOM** 234 CA VALA 20145.003 6.398 6.605 1.00 0.00 C **ATOM** ATOM 235 C VALA 20144.363 5.835 7.870 1.00 0.00 C **ATOM** 236 O VALA 20143.408 6.402 8.400 1.00 0.00 O 237 CB VALA 20146.035 7.470 7.000 1.00 0.00 C **ATOM** 238 CG1 VALA 20147.175 6.849 7.793 1.00 0.00 C **ATOM** ATOM 239 CG2 VAL A 20146.563 8.184 5.765 1.00 0.00 C 240 H VALA 20144.045 7.882 5.438 1.00 0.00 H **ATOM** 241 HA VALA 20145.520 5.603 6.089 1.00 0.00 H ATOM 242 HB VALA 20145.546 8.199 7.628 1.00 0.00 H **ATOM** 243 1HG1 VAL A 20146.826 6.589 8.781 1.00 0.00 H **ATOM** 244 2HG1 VAL A 20147.987 7.558 7.873 1.00 0.00 H ATOM **ATOM** 245 3HG1 VAL A 20147.523 5.960 7.289 1.00 0.00 H 246 1HG2 VAL A 20145.905 9.001 5.513 1.00 0.00 H ATOM 247 2HG2 VAL A 20146.608 7.489 4.939 1.00 0.00 H ATOM 248 3HG2 VAL A 20147.552 8.568 5.965 1.00 0.00 H ATOM ATOM 249 N GLY A 21144.897 4.714 8.348 1.00 0.00 N

250 CA GLY A 21144.365 4.094 9.547 1.00 0.00 C ATOM 251 C GLYA 21143.362 2.999 9.237 1.00 0.00 C 252 O GLY A 21143.332 1.968 9.909 1.00 0.00 O ATOM 253 H GLY A 21145.657 4.307 7.882 1.00 0.00 H ATOM · 254 1HA GLY A 21145.181 3.670 10.111 1.00 0.00 H 255 2HA GLY A 21143.881 4.850 10.147 1.00 0.00 H ATOM 256 N SER A 22142.540 3.222 8.216 1.00 0.00 N ATOM 257 CA SER A 22141.533 2.247 7.819 1.00 0.00 C ATOM **ATOM** 258 C SER A 22142.140 1.169 6.927 1.00 0.00 C ATOM 259 O SER A 22143.184 1.377 6.308 1.00 0.00 O **ATOM** 260 CB SER A 22140.381 2.940 7.088 1.00 0.00 C **ATOM** 261 OG SER A 22139.915 4.061 7.820 1.00 0.00 O **ATOM** 262 H SER A 22142.615 4.063 7.719 1.00 0.00 H ATOM 263 HA SER A 22141.150 1.782 8.716 1.00 0.00 H **ATOM** 264 1HB SER A 22140.722 3.275 6.120 1.00 0.00 H 265 2HB SER A 22139.566 2.244 6.962 1.00 0.00 H ATOM ATOM 266 HG SER A 22139.825 3.824 8.746 1.00 0.00 H ATOM 267 N LEUA 23141.480 0.017 6.867 1.00 0.00 N 268 CA LEU A 23141.956 -1.095 6.052 1.00 0.00 C ATOM **ATOM** 269 C LEUA 23141.365 -1.033 4.648 1.00 0.00 C 270 O LEUA 23140.256 -0.536 4.451 1.00 0.00 O ATOM 271 CB LEU A 23141.597 -2.428 6.711 1.00 0.00 C ATOM 272 CG LEUA 23142.398 -2.764 7.970 1.00 0.00 C ATOM 273 CD1 LEU A 23141.572 -3.626 8.913 1.00 0.00 C ATOM ATOM 274 CD2 LEU A 23143.697 -3.466 7.602 1.00 0.00 C 275 H LEU A 23140.655 -0.089 7.384 1.00 0.00 H ATOM 276 HA LEUA 23143.031 -1.017 5.981 1.00 0.00 H ATOM ATOM 277 1HB LEUA 23140.549 -2.406 6.971 1.00 0.00 H 278 2HB LEU A 23141.755 -3.216 5.990 1.00 0.00 H ATOM 279 HG LEU A 23142.646 -1.848 8.485 1.00 0.00 H ATOM 280 1HD1 LEU A 23141.798 -4.668 8.739 1.00 0.00 H

281 2HD1 LEU A 23140.522 -3.451 8.734 1.00 0.00 H ATOM 282 3HD1 LEU A 23141.817 -3.372 9.935 1.00 0.00 H ATOM 283 1HD2 LEU A 23144.307 -3.580 8.485 1.00 0.00 H 284 2HD2 LEU A 23144.230 -2.877 6.870 1.00 0.00 H ATOM 285 3HD2 LEU A 23143.475 -4.439 7.190 1.00 0.00 H ATOM **ATOM** 286 N ALAA 24142.112 -1.543 3.674 1.00 0.00 N 287 CA ALAA 24141.663 -1.547 2.287 1.00 0.00 C ATOM 288 C ALAA 24142.247 -2.733 1.526 1.00 0.00 C **ATOM** 289 O ALAA 24143.268 -3.294 1.920 1.00 0.00 O ATOM 290 CB ALAA 24142.041 -0.242 1.605 1.00 0.00 C **ATOM** 291 H ALAA 24142.987 -1.926 3.894 1.00 0.00 H ATOM 292 HA ALA A 24140.585 -1.627 2.286 1.00 0.00 H ATOM 293 1HB ALA A 24143.115 -0.194 1.488 1.00 0.00 H ATOM 294 2HB ALA A 24141.710 0.590 2.210 1.00 0.00 H ATOM 295 3HB ALA A 24141.571 -0.191 0.635 1.00 0.00 H ATOM 296 N GLUA 25141.590 -3.108 0.432 1.00 0.00 N ATOM 297 CA GLU A 25142.043 -4.228 -0.385 1.00 0.00 C **ATOM** 298 C GLUA 25142.350 -3.772 -1.808 1.00 0.00 C ATOM 299 O GLUA 25141.727 -2.844 -2.321 1.00 0.00 O **ATOM** 300 CB GLU A 25140.984 -5.332 -0.407 1.00 0.00 C ATOM 301 CG GLU A 25141.514 -6.676 -0.879 1.00 0.00 C **ATOM** 302 CD GLUA 25140.504 -7.441 -1.711 1.00 0.00 C **ATOM** 303 OE1 GLU A 25140.920 -8.347 -2.463 1.00 0.00 O **ATOM** 304 OE2 GLU A 25139.298 -7.134 -1.611 1.00 0.00 O **ATOM** 305 H GLU A 25140.781 -2.621 0.169 1.00 0.00 H **ATOM** 306 HA GLU A 25142.947 -4.617 0.058 1.00 0.00 H **ATOM** 307 1HB GLU A 25140.589 -5.454 0.590 1.00 0.00 H **ATOM** 308 2HB GLUA 25140.184 -5.032 -1.068 1.00 0.00 H **ATOM** 309 1HG GLUA 25142.399 -6.511 -1.476 1.00 0.00 H **ATOM ATOM** 310 2HG GLU A 25141.771 -7.270 -0.013 1.00 0.00 H ATOM 311 N VAL A 26143.315 -4.433 -2.442 1.00 0.00 N

- ATOM 312 CA VALA 26143.705 -4.095 -3.805 1.00 0.00 C
- ATOM 313 C VAL A 26143.324 -5.207 -4.777 1.00 0.00 C
- ATOM 314 O VALA 26143.308 -6.383 -4.414 1.00 0.00 O
- ATOM 315 CB VAL A 26145.219 -3.835 -3.909 1.00 0.00 C
- ATOM 316 CG1 VALA 26145.574 -3.289 -5.284 1.00 0.00 C
- ATOM 317 CG2 VAL A 26145.674 -2.882 -2.814 1.00 0.00 C
- ATOM 318 H VALA 26143.776 -5.165 -1.979 1.00 0.00 H
- ATOM 319 HA VAL A 26143.184 -3.191 -4.086 1.00 0.00 H
- ATOM 320 HB VALA 26145.735 -4.775 -3.776 1.00 0.00 H
- ATOM 321 1HG1 VAL A 26145.885 -4.100 -5.925 1.00 0.00 H
- ATOM 322 2HG1 VAL A 26146.379 -2.575 -5.190 1.00 0.00 H
- ATOM 323 3HG1 VAL A 26144.710 -2.802 -5.712 1.00 0.00 H
- ATOM 324 1HG2 VAL A 26145.138 -1.948 -2.905 1.00 0.00 H
- ATOM 325 2HG2 VAL A 26146.733 -2.700 -2.913 1.00 0.00 H
- ATOM 326 3HG2 VAL A 26145.472 -3.321 -1.849 1.00 0.00 H
- ATOM 327 N LYS A 27143.019 -4.827 -6.013 1.00 0.00 N
- ATOM 328 CA LYS A 27142.638 -5.792 -7.038 1.00 0.00 C
- ATOM 329 C LYS A 27143.856 -6.246 -7.835 1.00 0.00 C
- ATOM 330 O LYS A 27144.131 -5.728 -8.917 1.00 0.00 O
- ATOM 331 CB LYS A 27141.596 -5.184 -7.978 1.00 0.00 C
- ATOM 332 CG LYS A 27140.860 -6.215 -8.820 1.00 0.00 C
- ATOM 333 CD LYS A 27141.342 -6.206 -10.262 1.00 0.00 C
- ATOM 334 CE LYS A 27141.289 -7.596 -10.876 1.00 0.00 C
- ATOM 335 NZ LYS A 27141.792 -7.605 -12.277 1.00 0.00 N
- ATOM 336 H LYS A 27143.050 -3.875 -6.241 1.00 0.00 H
- ATOM 337 HA LYS A 27142.208 -6.649 -6.542 1.00 0.00 H
- ATOM 338 1HB LYS A 27140.867 -4.647 -7.389 1.00 0.00 H
- ATOM 339 2HB LYS A 27142.089 -4.491 -8.645 1.00 0.00 H
- ATOM 340 1HG LYS A 27141.031 -7.196 -8.400 1.00 0.00 H
- ATOM 341 2HG LYS A 27139.803 -5.993 -8.801 1.00 0.00 H
- ATOM 342 1HD LYS A 27140.712 -5.546 -10.838 1.00 0.00 H

343 2HD LYS A 27142.362 -5.850 -10.289 1.00 0.00 H ATOM 344 1HE LYS A 27141.897 -8.262 -10.281 1.00 0.00 H ATOM 345 2HE LYS A 27140.265 -7.940 -10.867 1.00 0.00 H **ATOM** 346 1HZ LYS A 27142.831 -7.630 -12.284 1.00 0.00 H 347 2HZ LYS A 27141.475 -6.749 -12.776 1.00 0.00 H ATOM ATOM 348 3HZ LYS A 27141.431 -8.439 -12.781 1.00 0.00 H 349 N GLUA 28144.583 -7.219 -7.294 1.00 0.00 N **ATOM** 350 CA GLUA 28145.772 -7.744 -7.955 1.00 0.00 C ATOM 351 C GLUA 28145.696 -9.263 -8.080 1.00 0.00 C ATOM 352 O GLUA 28144.649 -9.864 -7.844 1.00 0.00 O 353 CB GLUA 28147.030 -7.343 -7.180 1.00 0.00 C ATOM 354 CG GLUA 28148.126 -6.764 -8.060 1.00 0.00 C ATOM 355 CD GLUA 28148.802 -5.560 -7.433 1.00 0.00 C **ATOM** 356 OE1 GLU A 28149.942 -5.707 -6.944 1.00 0.00 O ATOM 357 OE2 GLU A 28148.191 -4.471 -7.431 1.00 0.00 O **ATOM** 358 H GLUA 28144.312 -7.593 -6.429 1.00 0.00 H **ATOM** 359 HA GLUA 28145.817 -7.315 -8.945 1.00 0.00 H **ATOM** 360 1HB GLU A 28146.763 -6.603 -6.441 1.00 0.00 H **ATOM** 361 2HB GLUA 28147.424 -8.215 -6.678 1.00 0.00 H **ATOM** 362 1HG GLUA 28148.871 -7.526 -8.233 1.00 0.00 H ATOM 363 2HG GLUA 28147.693 -6.465 -9.003 1.00 0.00 H **ATOM** 364 N ASNA 29146.815 -9.877 -8.453 1.00 0.00 N **ATOM** 365 CA ASN A 29146.875 -11.325 -8.608 1.00 0.00 C **ATOM** 366 C ASN A 29146.931 -12.016 -7.247 1.00 0.00 C ATOM 367 O ASN A 29146.068 -12.831 -6.920 1.00 0.00 O ATOM 368 CB ASN A 29148.093 -11.719 -9.448 1.00 0.00 C **ATOM** 369 CG ASN A 29147.735 -11.979 -10.898 1.00 0.00 C **ATOM** 370 OD1 ASN A 29147.584 -13.127 -11.316 1.00 0.00 O ATOM 371 ND2 ASN A 29147.598 -10.910 -11.674 1.00 0.00 N ATOM **ATOM** 372 H ASNA 29147.619 -9.344 -8.626 1.00 0.00 H ATOM 373 HA ASN A 29145.978 -11.640 -9.121 1.00 0.00 H

374 1HB ASN A 29148.819 -10.921 -9.413 1.00 0.00 H **ATOM** 375 2HB ASN A 29148.531 -12.617 -9.037 1.00 0.00 H **ATOM** 376 1HD2 ASN A 29147.734 -10.027 -11.273 1.00 0.00 H **ATOM ATOM** 377 2HD2 ASN A 29147.368 -11.049 -12.616 1.00 0.00 H 378 N PRO A 30147.953 -11.697 -6.434 1.00 0.00 N **ATOM** 379 CA PRO A 30148.120 -12.289 -5.105 1.00 0.00 C **ATOM** 380 C PRO A 30147.205 -11.646 -4.063 1.00 0.00 C **ATOM** 381 O PRO A 30147.389 -10.485 -3.701 1.00 0.00 O **ATOM** 382 CB PRO A 30149.583 -11.995 -4.782 1.00 0.00 C **ATOM** 383 CG PRO A 30149.872 -10.721 -5.497 1.00 0.00 C **ATOM** 384 CD PRO A 30149.028 -10.735 -6.746 1.00 0.00 C ATOM 385 HA PRO A 30147.959 -13.357 -5.123 1.00 0.00 H ATOM 386 1HB PRO A 30149.705 -11.890 -3.714 1.00 0.00 H **ATOM** 387 2HB PRO A 30150.205 -12.800 -5.145 1.00 0.00 H ATOM 388 1HG PRO A 30149.602 -9.881 -4.872 1.00 0.00 H **ATOM** 389 2HG PRO A 30150.920 -10.674 -5.754 1.00 0.00 H **ATOM** 390 1HD PRO A 30148.621 -9.752 -6.936 1.00 0.00 H **ATOM** 391 2HD PRO A 30149.612 -11.070 -7.590 1.00 0.00 H **ATOM** 392 N PRO A 31146.201 -12.393 -3.566 1.00 0.00 N **ATOM** 393 CA PRO A 31145.261 -11.880 -2.562 1.00 0.00 C ATOM 394 C PRO A 31145.954 -11.524 -1.252 1.00 0.00 C **ATOM** 395 O PRO A 31146.396 -12.403 -0.513 1.00 0.00 O ATOM 396 CB PRO A 31144.280 -13.041 -2.347 1.00 0.00 C **ATOM** 397 CG PRO A 31144.464 -13.934 -3.527 1.00 0.00 C **ATOM** 398 CD PRO A 31145.900 -13.784 -3.937 1.00 0.00 C **ATOM** ATOM 399 HA PRO A 31144.725 -11.017 -2.930 1.00 0.00 H 400 1HB PRO A 31144.523 -13.553 -1.427 1.00 0.00 H ATOM 401 2HB PRO A 31143.272 -12.660 -2.297 1.00 0.00 H ATOM 402 1HG PRO A 31144.257 -14.958 -3.251 1.00 0.00 H ATOM

403 2HG PRO A 31143.812 -13.622 -4.330 1.00 0.00 H

404 1HD PRO A 31146.524 -14.474 -3.389 1.00 0.00 H

ATOM

ATOM

- ATOM 405 2HD PRO A 31146.009 -13.933 -5.000 1.00 0.00 H
- ATOM 406 N PHE A 32146.045 -10.228 -0.969 1.00 0.00 N
- ATOM 407 CA PHE A 32146.685 -9.757 0.254 1.00 0.00 C
- ATOM 408 C PHE A 32145.819 -8.715 0.955 1.00 0.00 C
- ATOM 409 O .PHE A 32144.887 -8.169 0.365 1.00 0.00 O
- ATOM 410 CB PHE A 32148.062 -9.169 -0.058 1.00 0.00 C
- ATOM 411 CG PHE A 32148.060 -8.215 -1.219 1.00 0.00 C
- ATOM 412 CD1 PHE A 32148.759 -8.514 -2.377 1.00 0.00 C
- ATOM 413 CD2 PHE A 32147.362 -7.020 -1.150 1.00 0.00 C
- ATOM 414 CE1 PHE A 32148.759 -7.640 -3.448 1.00 0.00 C
- ATOM 415 CE2 PHE A 32147.359 -6.142 -2.217 1.00 0.00 C
- ATOM 416 CZ PHE A 32148.059 -6.452 -3.368 1.00 0.00 C
- ATOM 417 H PHE A 32145.674 -9.573 -1.596 1.00 0.00 H
- ATOM 418 HA PHE A 32146.807 -10.605 0.911 1.00 0.00 H
- ATOM 419 1HB PHE A 32148.421 -8.635 0.809 1.00 0.00 H
- ATOM 420 2HB PHE A 32148.746 -9.973 -0.287 1.00 0.00 H
- ATOM 421 HD1 PHE A 32149.306 -9.443 -2.442 1.00 0.00 H
- ATOM 422 HD2 PHE A 32146.815 -6.776 -0.252 1.00 0.00 H
- ATOM 423 HE1 PHE A 32149.308 -7.885 -4.346 1.00 0.00 H
- ATOM 424 HE2 PHE A 32146.811 -5.213 -2.153 1.00 0.00 H
- ATOM 425 HZ PHE A 32148.059 -5.767 -4.202 1.00 0.00 H
- ATOM 426 N TYR A 33146.135 -8.443 2.217 1.00 0.00 N
- ATOM 427 CA TYR A 33145.387 -7.466 2.999 1.00 0.00 C
- ATOM 428 C TYR A 33146.331 -6.522 3.736 1.00 0.00 C
- ATOM 429 O TYR A 33147.344 -6.948 4.290 1.00 0.00 O
- ATOM 430 CB TYR A 33144.472 -8.176 3.999 1.00 0.00 C
- ATOM 431 CG TYR A 33143.246 -8.794 3.366 1.00 0.00 C
- ATOM 432 CD1 TYR A 33142.976 -10.149 3.508 1.00 0.00 C
- ATOM 433 CD2 TYR A 33142.360 -8.023 2.625 1.00 0.00 C
- ATOM 434 CE1 TYR A 33141.857 -10.718 2.931 1.00 0.00 C
- ATOM 435 CE2 TYR A 33141.238 -8.584 2.045 1.00 0.00 C

436 CZ TYR A 33140.992 -9.931 2.200 1.00 0.00 C ATOM 437 OH TYR A 33139.875 -10.494 1.624 1.00 0.00 O ATOM 438 H TYR A 33146.890 -8.911 2.633 1.00 0.00 H 439 HA TYR A 33144.781 -6.890 2.316 1.00 0.00 H **ATOM** 440 1HB TYR A 33145.026 -8.963 4.486 1.00 0.00 H **ATOM** 441 2HB TYR A 33144.141 -7.464 4.740 1.00 0.00 H **ATOM ATOM** 442 HD1 TYR A 33143.656 -10.763 4.081 1.00 0.00 H ATOM 443 HD2 TYR A 33142.556 -6.968 2.505 1.00 0.00 H **ATOM** 444 HE1 TYR A 33141.663 -11.774 3.053 1.00 0.00 H 445 HE2 TYR A 33140.561 -7.968 1.472 1.00 0.00 H **ATOM** ATOM 446 HH TYR A 33140.098 -11.360 1.275 1.00 0.00 H 447 N GLYA 34145.991 -5.237 3.739 1.00 0.00 N **ATOM ATOM** 448 CA GLY A 34146.818 -4.253 4.412 1.00 0.00 C 449 C GLY A 34146.029 -3.038 4.858 1.00 0.00 C ATOM 450 O GLY A 34144.844 -2.911 4.549 1.00 0.00 O ATOM 451 H GLY A 34145.172 -4.955 3.281 1.00 0.00 H **ATOM** 452 1HA GLY A 34147.272 -4.712 5.278 1.00 0.00 H **ATOM** ATOM 453 2HA GLY A 34147.599 -3.933 3.737 1.00 0.00 H 454 N VALA 35146.687 -2.143 5.588 1.00 0.00 N ATOM 455 CA VALA 35146.038 -0.932 6.079 1.00 0.00 C ATOM 456 C VALA 35146.696 0.316 5.500 1.00 0.00 C ATOM 457 O VALA 35147.920 0.388 5.382 1.00 0.00 O **ATOM** 458 CB VALA 35146.078 -0.860 7.619 1.00 0.00 C **ATOM** 459 CG1 VAL A 35147.514 -0.810 8.119 1.00 0.00 C **ATOM** 460 CG2 VAL A 35145,288 0.341 8.119 1.00 0.00 C ATOM 461 H VALA 35147.629 -2.300 5.802 1.00 0.00 H **ATOM** 462 HA VALA 35145.004 -0.959 5.767 1.00 0.00 H ATOM 463 HB VALA 35145.616 -1.754 8.012 1.00 0.00 H **ATOM** 464 1HG1 VAL A 35147.617 -1.449 8.984 1.00 0.00 H ATOM 465 2HG1 VAL A 35147.765 0.205 8.391 1.00 0.00 H ATOM 466 3HG1 VAL A 35148.179 -1.148 7.339 1.00 0.00 H ATOM

467 1HG2 VAL A 35144.239 0.197 7.903 1.00 0.00 H ATOM **ATOM** 468 2HG2 VAL A 35145.637 1.234 7.622 1.00 0.00 H 469 3HG2 VAL A 35145.425 0.444 9.185 1.00 0.00 H **ATOM** 470 N ILE A 36145.876 1.300 5.143 1.00 0.00 N ATOM 471 CA ILE A 36146.379 2.546 4.577 1.00 0.00 C ATOM 472 C ILE A 36147.308 3.255 5.558 1.00 0.00 C **ATOM** ATOM 473 O ILE A 36147.020 3.340 6.751 1.00 0.00 O ATOM 474 CB ILE A 36145.228 3.498 4.194 1.00 0.00 C 475 CG1 ILE A 36144.210 2.776 3.308 1.00 0.00 C 476 CG2 ILE A 36145.772 4.732 3.486 1.00 0.00 C ATOM 477 CD1 ILE A 36143.058 3.654 2.872 1.00 0.00 C **ATOM** ATOM 478 H ILE A 36144.911 1.184 5.262 1.00 0.00 H ATOM 479 HA ILE A 36146.934 2.305 3.681 1.00 0.00 H 480 HB ILE A 36144.741 3.820 5.102 1.00 0.00 H ATOM 481 1HG1 ILE A 36144.706 2.416 2.420 1.00 0.00 H ATOM 482 2HG1 ILE A 36143.801 1.936 3.852 1.00 0.00 H ATOM 483 1HG2 ILE A 36145.242 5.607 3.832 1.00 0.00 H ATOM ATOM 484 2HG2 ILE A 36145.632 4.626 2.420 1.00 0.00 H 485 3HG2 ILE A 36146.824 4.838 3.702 1.00 0.00 H **ATOM** 486 1HD1 ILE A 36142.131 3.246 3.251 1.00 0.00 H ATOM 487 2HD1 ILE A 36143.021 3.690 1.794 1.00 0.00 H ATOM 488 3HD1 ILE A 36143.197 4.651 3.263 1.00 0.00 H **ATOM** 489 N ARG A 37148.425 3.761 5.045 1.00 0.00 N ATOM **ATOM** 490 CA ARG A 37149.398 4.463 5.876 1.00 0.00 C 491 C ARG A 37149.620 5.885 5.372 1.00 0.00 C **ATOM** 492 O ARG A 37149.301 6.854 6.060 1.00 0.00 O ATOM 493 CB ARG A 37150.725 3.703 5.895 1.00 0.00 C ATOM 494 CG ARG A 37150.572 2.216 6.176 1.00 0.00 C ATOM 495 CD ARG A 37150.497 1.937 7.668 1.00 0.00 C ATOM 496 NE ARG A 37149.266 2.455 8.261 1.00 0.00 N ATOM ATOM 497 CZ ARG A 37149.103 2.662 9.566 1.00 0.00 C

498 NH1 ARG A 37150.087 2.396 10.417 1.00 0.00 N ATOM **ATOM** 499 NH2 ARG A 37147.951 3.135 10.023 1.00 0.00 N 500 H ARG A 37148.601 3.660 4.086 1.00 0.00 H ATOM 501 HA ARG A 37149.005 4.507 6.880 1.00 0.00 H ATOM 502 1HB ARG A 37151.206 3.817 4.934 1.00 0.00 H ATOM 503 2HB ARG A 37151.359 4.128 6.658 1.00 0.00 H ATOM 504 1HG ARG A 37149.665 1.864 5.709 1.00 0.00 H ATOM 505 2HG ARG A 37151.421 1.692 5.762 1.00 0.00 H ATOM **ATOM** 506 1HD ARG A 37150.539 0.870 7.824 1.00 0.00 H 507 2HD ARG A 37151.343 2.404 8.151 1.00 0.00 H ATOM 508 HE ARG A 37148.523 2.659 7.656 1.00 0.00 H ATOM 509 1HH1 ARG A 37150.957 2.038 10.079 1.00 0.00 H **ATOM** 510 2HH1 ARG A 37149.958 2.554 11.395 1.00 0.00 H ATOM 511 1HH2 ARG A 37147.206 3.338 9.387 1.00 0.00 H ATOM 512 2HH2 ARG A 37147.828 3.291 11.003 1.00 0.00 H **ATOM** 513 N TRPA 38150.168 6.003 4.168 1.00 0.00 N ATOM 514 CA TRP A 38150.433 7.308 3.573 1.00 0.00 C **ATOM** ATOM 515 C TRPA 38149.677 7.472 2.256 1.00 0.00 C 516 O TRPA 38149.724 6.600 1.389 1.00 0.00 O **ATOM** 517 CB TRP A 38151.937 7.494 3.343 1.00 0.00 C **ATOM** 518 CG TRPA 38152.271 8.679 2.486 1.00 0.00 C **ATOM** 519 CD1 TRP A 38152.549 9.947 2.909 1.00 0.00 C **ATOM** 520 CD2 TRP A 38152.356 8.706 1.056 1.00 0.00 C ATOM 521 NE1 TRP A 38152.802 10.760 1.830 1.00 0.00 N **ATOM** 522 CE2 TRP A 38152.689 10.021 0.681 1.00 0.00 C ATOM 523 CE3 TRP A 38152.183 7.745 0.057 1.00 0.00 C **ATOM** 524 CZ2 TRP A 38152.852 10.398 -0.650 1.00 0.00 C ATOM 525 CZ3 TRP A 38152.345 8.119 -1.263 1.00 0.00 C ATOM 526 CH2 TRP A 38152.676 9.435 -1.607 1.00 0.00 C ATOM 527 H TRP A 38150.401 5.193 3.666 1.00 0.00 H ATOM ATOM 528 HA TRP A 38150.089 8.062 4.266 1.00 0.00 H

529 1HB TRPA 38152.427 7.624 4.296 1.00 0.00 H ATOM 530 2HB TRP A 38152.331 6.611 2.860 1.00 0.00 H **ATOM** 531 HD1 TRP A 38152.564 10.253 3.945 1.00 0.00 H ATOM 532 HE1 TRP A 38153.026 11.713 1.876 1.00 0.00 H 533 HE3 TRP A 38151.927 6.725 0.301 1.00 0.00 H **ATOM** 534 HZ2 TRP A 38153.105 11.409 -0.931 1.00 0.00 H ATOM ATOM 535 HZ3 TRP A 38152.214 7.389 -2.050 1.00 0.00 H 536 HH2 TRP A 38152.793 9.683 -2.653 1.00 0.00 H ATOM **ATOM** 537 N ILE A 39148.993 8.601 2.114 1.00 0.00 N 538 CA ILE A 39148.236 8.890 0.902 1.00 0.00 C **ATOM** 539 C ILE A 39148.716 10.190 0.268 1.00 0.00 C **ATOM** 540 O ILE A 39148.434 11.278 0.771 1.00 0.00 O **ATOM** 541 CB ILE A 39146.726 8.999 1.193 1.00 0.00 C **ATOM** 542 CG1 ILE A 39146.253 7.793 2.006 1.00 0.00 C ATOM 543 CG2 ILE A 39145.943 9.110 -0.106 1.00 0.00 C **ATOM** 544 CD1 ILE A 39144.821 7.908 2.482 1.00 0.00 C ATOM 545 H ILE A 39149.002 9.259 2.839 1.00 0.00 H **ATOM ATOM** 546 HA ILE A 39148.392 8.079 0.207 1.00 0.00 H 547 HB ILE A 39146.556 9.898 1.765 1.00 0.00 H **ATOM** 548 1HG1 ILE A 39146.329 6.904 1.398 1.00 0.00 H **ATOM** 549 2HG1 ILE A 39146.885 7.682 2.876 1.00 0.00 H ATOM 550 1HG2 ILE A 39146.511 8.664 -0.909 1.00 0.00 H **ATOM** 551 2HG2 ILE A 39145.761 10.151 -0.328 1.00 0.00 H **ATOM** 552 3HG2 ILE A 39145.000 8.593 -0.003 1.00 0.00 H ATOM 553 1HD1 ILE A 39144.804 8.363 3.462 1.00 0.00 H **ATOM** 554 2HD1 ILE A 39144.379 6.925 2.534 1.00 0.00 H **ATOM** 555 3HD1 ILE A 39144.261 8.520 1.790 1.00 0.00 H ATOM 556 N GLY A 40149.446 10.073 -0.836 1.00 0.00 N **ATOM** 557 CA GLY A 40149.956 11.250 -1.512 1.00 0.00 C ATOM 558 C GLY A 40150.450 10.954 -2.913 1.00 0.00 C ATOM 559 O GLY A 40150.200 9.877 -3.455 1.00 0.00 O ATOM

560 H GLYA 40149.644 9.181 -1.192 1.00 0.00 H **ATOM** 561 1HA GLY A 40149.172 11.988 -1.567 1.00 0.00 H **ATOM** 562 2HA GLY A 40150.774 11.655 -0.934 1.00 0.00 H ATOM 563 N GLNA 41151.151 11.918 -3.503 1.00 0.00 N **ATOM** 564 CA GLN A 41151.682 11.767 -4.850 1.00 0.00 C **ATOM** 565 C GLN A 41153.178 12.077 -4.881 1.00 0.00 C **ATOM ATOM** 566 O GLN A 41153.587 13.211 -4.627 1.00 0.00 O 567 CB GLN A 41150.936 12.694 -5.810 1.00 0.00 C **ATOM ATOM** 568 CG GLN A 41149.424 12.612 -5.681 1.00 0.00 C 569 CD GLNA 41148.756 13.969 -5.779 1.00 0.00 C **ATOM** 570 OE1 GLN A 41148.808 14.769 -4.846 1.00 0.00 O **ATOM** ATOM 571 NE2 GLN A 41148.124 14.235 -6.916 1.00 0.00 N 572 H GLN A 41151.313 12.753 -3.019 1.00 0.00 H ATOM 573 HA GLN A 41151.527 10.744 -5.158 1.00 0.00 H ATOM **ATOM** 574 1HB GLN A 41151.236 13.711 -5.614 1.00 0.00 H 575 2HB GLN A 41151.205 12.436 -6.822 1.00 0.00 H ATOM 576 1HG GLN A 41149.040 11.982 -6.470 1.00 0.00 H ATOM 577 2HG GLN A 41149.179 12.175 -4.724 1.00 0.00 H ATOM 578 1HE2 GLN A 41148.124 13.549 -7.616 1.00 0.00 H **ATOM** 579 2HE2 GLN A 41147.685 15.106 -7.009 1.00 0.00 H **ATOM** 580 N PRO A 42154.020 11.075 -5.191 1.00 0.00 N ATOM 581 CA PRO A 42155.475 11.257 -5.248 1.00 0.00 C **ATOM** 582 C PRO A 42155.883 12.348 -6.233 1.00 0.00 C **ATOM** 583 O PRO A 42155.116 12.706 -7.128 1.00 0.00 O **ATOM** 584 CB PRO A 42155.994 9.893 -5.715 1.00 0.00 C **ATOM** 585 CG PRO A 42154.914 8.931 -5.358 1.00 0.00 C **ATOM** 586 CD PRO A 42153.628 9.690 -5.508 1.00 0.00 C ATOM 587 HA PRO A 42155.882 11.485 -4.274 1.00 0.00 H **ATOM** 588 1HB PRO A 42156.167 9.916 -6.781 1.00 0.00 H ATOM 589 2HB PRO A 42156.914 9.659 -5.200 1.00 0.00 H **ATOM** 590 1HG PRO A 42154.933 8.088 -6.033 1.00 0.00 H **ATOM**

591 2HG PRO A 42155.037 8.600 -4.338 1.00 0.00 H ATOM 592 1HD PRO A 42153.259 9.615 -6.520 1.00 0.00 H ATOM 593 2HD PRO A 42152.890 9.327 -4.806 1.00 0.00 H ATOM 594 N PRO A 43157.103 12.891 -6.082 1.00 0.00 N **ATOM** 595 CA PRO A 43157.611 13.946 -6.963 1.00 0.00 C ATOM 596 C PRO A 43157.953 13.424 -8.354 1.00 0.00 C ATOM ATOM 597 O PRO A 43159.092 13.042 -8.621 1.00 0.00 O 598 CB PRO A 43158.874 14.427 -6.250 1.00 0.00 C ATOM 599 CG PRO A 43159.327 13.252 -5.454 1.00 0.00 C ATOM 600 CD PRO A 43158.079 12.520 -5.041 1.00 0.00 C ATOM 601 HA PRO A 43156.908 14.763 -7.049 1.00 0.00 H ATOM ATOM 602 1HB PRO A 43159.613 14.718 -6.982 1.00 0.00 H 603 2HB PRO A 43158.636 15.266 -5.615 1.00 0.00 H **ATOM** 604 1HG PRO A 43159.951 12.615 -6.063 1.00 0.00 H ATOM 605 2HG PRO A 43159.871 13.587 -4.583 1.00 0.00 H ATOM 606 1HD PRO A 43158.252 11.454 -5.037 1.00 0.00 H **ATOM** 607 2HD PRO A 43157.751 12.855 -4.068 1.00 0.00 H **ATOM** 608 N GLY A 44156.960 13.410 -9.236 1.00 0.00 N **ATOM** 609 CA GLY A 44157.179 12.932 -10.588 1.00 0.00 C ATOM 610 C GLYA 44155.901 12.471 -11.257 1.00 0.00 C ATOM 611 O GLY A 44155.595 12.885 -12.375 1.00 0.00 O ATOM 612 H GLY A 44156.072 13.725 -8.968 1.00 0.00 H ATOM 613 1HA GLY A 44157.612 13.728 -11.173 1.00 0.00 H ATOM ATOM 614 2HA GLY A 44157.875 12.105 -10.556 1.00 0.00 H 615 N LEUA 45155.154 11.611 -10.574 1.00 0.00 N **ATOM** 616 CA LEU A 45153.902 11.095 -11.112 1.00 0.00 C **ATOM** 617 C LEUA 45152.735 11.431 -10.190 1.00 0.00 C ATOM 618 O LEUA 45152.647 10.916 -9.076 1.00 0.00 O ATOM 619 CB LEUA 45153.993 9.580 -11.306 1.00 0.00 C ATOM 620 CG LEUA 45154.530 8.806 -10.099 1.00 0.00 C **ATOM** 621 CD1 LEU A 45154.083 7.352 -10.154 1.00 0.00 C ATOM

- ATOM 622 CD2 LEU A 45156.049 8.900 -10.039 1.00 0.00 C
- ATOM 623 H LEU A 45155.450 11.319 -9.685 1.00 0.00 H
- ATOM 624 HA LEU A 45153.734 11.562 -12.070 1.00 0.00 H
- ATOM 625 1HB LEU A 45153.006 9.208 -11.537 1.00 0.00 H
- ATOM 626 2HB LEU A 45154.640 9.384 -12.147 1.00 0.00 H
- ATOM 627 HG LEU A 45154.131 9.243 -9.196 1.00 0.00 H
- ATOM 628 1HD1 LEU A 45153.399 7.155 -9.341 1.00 0.00 H
- ATOM 629 2HD1 LEU A 45154.943 6.705 -10.064 1.00 0.00 H
- ATOM 630 3HD1 LEU A 45153.587 7.161 -11.094 1.00 0.00 H
- ATOM 631 1HD2 LEU A 45156.481 7.939 -10.273 1.00 0.00 H
- ATOM 632 2HD2 LEU A 45156.351 9.197 -9.044 1.00 0.00 H
- ATOM 633 3HD2 LEU A 45156.395 9.634 -10.752 1.00 0.00 H
- ATOM 634 N ASN A 46151.839 12.293 -10.660 1.00 0.00 N
- ATOM 635 CA ASN A 46150.682 12.685 -9.866 1.00 0.00 C
- ATOM 636 C ASN A 46149.666 11.550 -9.807 1.00 0.00 C
- ATOM 637 O ASN A 46148.992 11.253 -10.792 1.00 0.00 O
- . ATOM 638 CB ASN A 46150.034 13.937 -10.460 1.00 0.00 C
- ATOM 639 CG ASN A 46149.364 14.797 -9.406 1.00 0.00 C
- ATOM 640 OD1 ASN A 46149.991 15.199 -8.426 1.00 0.00 O
- ATOM 641 ND2 ASN A 46148.083 15.083 -9.604 1.00 0.00 N
- ATOM 642 H ASN A 46151.958 12.670 -11.556 1.00 0.00 H
- ATOM 643 HA ASN A 46151.023 12.904 -8.865 1.00 0.00 H
- ATOM 644 1HB ASN A 46150.792 14.529 -10.950 1.00 0.00 H
- ATOM 645 2HB ASN A 46149.290 13.640 -11.184 1.00 0.00 H
- ATOM 646 1HD2 ASN A 46147.648 14.729 -10.408 1.00 0.00 H
- ATOM 647 2HD2 ASN A 46147.625 15.639 -8.939 1.00 0.00 H
- ATOM 648 N GLU A 47149.563 10.920 -8.642 1.00 0.00 N
- ATOM 649 CA GLU A 47148.631 9.817 -8.447 1.00 0.00 C
- ATOM 650 C GLUA 47148.480 9.494 -6.965 1.00 0.00 C
- ATOM 651 O GLUA 47149.455 9.161 -6.291 1.00 0.00 O
- ATOM 652 CB GLU A 47149.104 8.574 -9.206 1.00 0.00 C

- ATOM 653 CG GLU A 47150.611 8.372 -9.178 1.00 0.00 C
- ATOM 654 CD GLU A 47151.090 7.413 -10.250 1.00 0.00 C
- ATOM 655 OE1 GLU A 47151.384 6.246 -9.915 1.00 0.00 O
- ATOM 656 OE2 GLU A 47151.171 7.829 -11.425 1.00 0.00 O
- ATOM 657 H GLUA 47150.130 11.205 -7.896 1.00 0.00 H
- ATOM 658 HA GLU A 47147.671 10.122 -8.836 1.00 0.00 H
- ATOM 659 1HB GLU A 47148.638 7.703 -8.771 1.00 0.00 H
- ATOM 660 2HB GLU A 47148.793 8.658 -10.237 1.00 0.00 H
- ATOM 661 1HG GLU A 47151.093 9.326 -9.329 1.00 0.00 H
- ATOM 662 2HG GLU A 47150.892 7.978 -8.212 1.00 0.00 H
- ATOM 663 N VALA 48147.255 9.585 -6.461 1.00 0.00 N
- ATOM 664 CA VALA 48146.988 9.294 -5.059 1.00 0.00 C
- ATOM 665 C VALA 48147.302 7.836 -4.743 1.00 0.00 C
- ATOM 666 O VALA 48146.505 6.943 -5.029 1.00 0.00 O
- ATOM 667 CB VALA 48145.522 9.585 -4.689 1.00 0.00 C
- ATOM 668 CG1 VAL A 48145.318 9.474 -3.186 1.00 0.00 C
- ATOM 669 CG2 VAL A 48145.108 10.959 -5.192 1.00 0.00 C
- ATOM 670 H VALA 48146.514 9.850 -7.045 1.00 0.00 H
- ATOM 671 HA VALA 48147.625 9.928 -4.458 1.00 0.00 H
- ATOM 672 HB VAL A 48144.897 8.846 -5.169 1.00 0.00 H
- ATOM 673 1HG1 VAL A 48145.394 8.440 -2.887 1.00 0.00 H
- ATOM 674 2HG1 VAL A 48144.339 9.853 -2.928 1.00 0.00 H
- ATOM 675 3HG1 VAL A 48146.073 10.054 -2.677 1.00 0.00 H
- ATOM 676 1HG2 VAL A 48144.413 11.403 -4.495 1.00 0.00 H
- ATOM 677 2HG2 VAL A 48144.636 10.861 -6.158 1.00 0.00 H
- ATOM 678 3HG2 VAL A 48145.981 11.589 -5.280 1.00 0.00 H
- ATOM 679 N LEUA 49148.472 7.601 -4.156 1.00 0.00 N
- ATOM 680 CA LEU A 49148.892 6.250 -3.807 1.00 0.00 C
- ATOM 681 C LEU A 49148.847 6.042 -2.299 1.00 0.00 C
- ATOM 682 O LEUA 49149.562 6.707 -1.549 1.00 0.00 O
- ATOM 683 CB LEU A 49150.306 5.982 -4.327 1.00 0.00 C

684 CG LEUA 49150.455 6.034 -5.849 1.00 0.00 C **ATOM** 685 CD1 LEU A 49151.876 6.420 -6.232 1.00 0.00 C **ATOM** 686 CD2 LEU A 49150.080 4.696 -6.467 1.00 0.00 C **ATOM ATOM** 687 H LEUA 49149.066 8.354 -3.954 1.00 0.00 H ATOM 688 HA LEU A 49148.208 5.558 -4.274 1.00 0.00 H 689 1HB LEU A 49150.971 6.715 -3.896 1.00 0.00 H ATOM 690 2HB LEU A 49150.610 5.002 -3.992 1.00 0.00 H ATOM 691 HG LEU A 49149.787 6.786 -6.245 1.00 0.00 H **ATOM** 692 1HD1 LEU A 49152.135 7.354 -5.757 1.00 0.00 H **ATOM** 693 2HD1 LEU A 49151.942 6.530 -7.304 1.00 0.00 H **ATOM** 694 3HD1 LEU A 49152.559 5.649 -5.906 1.00 0.00 H **ATOM** 695 1HD2 LEU A 49149.173 4.330 -6.007 1.00 0.00 H **ATOM** 696 2HD2 LEU A 49150.878 3.987 -6.303 1.00 0.00 H **ATOM** 697 3HD2 LEU A 49149.920 4.821 -7.527 1.00 0.00 H ATOM **ATOM** 698 N ALAA 50148.001 5.118 -1.861 1.00 0.00 N 699 CA ALAA 50147.865 4.827 -0.441 1.00 0.00 C ATOM 700 C ALAA 50148.802 3.700 -0.019 1.00 0.00 C **ATOM** ATOM 701 O ALAA 50148.655 2.561 -0.462 1.00 0.00 O **ATOM** 702 CB ALAA 50146.423 4.471 -0.111 1.00 0.00 C 703 H ALAA 50147.456 4.621 -2.506 1.00 0.00 H ATOM 704 HA ALAA 50148.124 5.723 0.106 1.00 0.00 H **ATOM** 705 1HB ALAA 50146.405 3.738 0.682 1.00 0.00 H **ATOM** 706 2HB ALA A 50145.943 4.063 -0.988 1.00 0.00 H **ATOM ATOM** 707 3HB ALAA 50145.896 5.358 0.208 1.00 0.00 H 708 N GLY A 51149.764 4.024 0.838 1.00 0.00 N **ATOM ATOM** 709 CA GLY A 51150.710 3.029 1.304 1.00 0.00 C 710 C GLYA 51150.071 2.011 2.229 1.00 0.00 C **ATOM** 711 O GLYA 51149.790 2.310 3.390 1.00 0.00 O **ATOM ATOM** 712 H GLY A 51149.832 4.950 1.156 1.00 0.00 H 713 1HA GLY A 51151.122 2.512 0.450 1.00 0.00 H **ATOM** 714 2HA GLY A 51151.510 3.526 1.830 1.00 0.00 H ATOM

715 N LEUA 52149.841 0.808 1.715 1.00 0.00 N 716 CA LEU A 52149.231 -0.256 2.503 1.00 0.00 C **ATOM ATOM** 717 C LEUA 52150.296 -1.119 3.171 1.00 0.00 C 718 O LEUA 52151.352 -1.377 2.594 1.00 0.00 O **ATOM** 719 CB LEUA 52148.333 -1.124 1.619 1.00 0.00 C **ATOM** 720 CG LEUA 52147.158 -0.390 0.972 1.00 0.00 C **ATOM ATOM** 721 CD1 LEU A 52146.581 -1.211 -0.171 1.00 0.00 C **ATOM** 722 CD2 LEU A 52146.085 -0.087 2.006 1.00 0.00 C **ATOM** 723 H LEU A 52150.088 0.631 0.782 1.00 0.00 H 724 HA LEUA 52148.627 0.206 3.271 1.00 0.00 H **ATOM** 725 1HB LEUA 52148.942 -1.551 0.835 1.00 0.00 H **ATOM** 726 2HB LEU A 52147.938 -1.928 2.223 1.00 0.00 H **ATOM** 727 HG LEU A 52147.507 0.548 0.565 1.00 0.00 H **ATOM** 728 1HD1 LEU A 52145.819 -1.874 0.211 1.00 0.00 H **ATOM** 729 2HD1 LEU A 52147.367 -1.793 -0.630 1.00 0.00 H **ATOM** 730 3HD1 LEU A 52146.147 -0.550 -0.906 1.00 0.00 H ATOM 731 1HD2 LEU A 52145.114 -0.103 1.534 1.00 0.00 H **ATOM ATOM** 732 2HD2 LEU A 52146.261 0.891 2.432 1.00 0.00 H 733 3HD2 LEU A 52146.118 -0.831 2.789 1.00 0.00 H **ATOM** 734 N GLUA 53150.010 -1.565 4.390 1.00 0.00 N **ATOM** 735 CA GLUA 53150.943 -2.400 5.137 1.00 0.00 C **ATOM** 736 C GLUA 53150.426 -3.831 5.244 1.00 0.00 C **ATOM** 737 O GLUA 53149.452 -4.099 5.948 1.00 0.00 O **ATOM** 738 CB GLUA 53151.171 -1.823 6.535 1.00 0.00 C **ATOM** 739 CG GLUA 53152.170 -2.613 7.365 1.00 0.00 C **ATOM** 740 CD GLUA 53151.776 -2.697 8.827 1.00 0.00 C **ATOM** 741 OE1 GLU A 53152.274 -3.607 9.524 1.00 0.00 O ATOM 742 OE2 GLU A 53150.970 -1.856 9.275 1.00 0.00 O **ATOM** 743 H GLUA 53149.151 -1.326 4.797 1.00 0.00 H ATOM 744 HA GLUA 53151.882 -2.409 4.604 1.00 0.00 H **ATOM** 745 1HB GLUA 53151.536 -0.811 6.440 1.00 0.00 H ATOM

746 2HB GLUA 53150.229 -1.809 7.064 1.00 0.00 H **ATOM** ATOM 747 1HG GLU A 53152.236 -3.615 6.968 1.00 0.00 H 748 2HG GLUA 53153.135 -2.134 7.295 1.00 0.00 H **ATOM ATOM** 749 N LEUA 54151.083 -4.747 4.540 1.00 0.00 N 750 CA LEU A 54150.690 -6.152 4.556 1.00 0.00 C ATOM 751 C LEUA 54150.936 -6.770 5.929 1.00 0.00 C **ATOM** 752 O LEUA 54151.987 -6.563 6.535 1.00 0.00 O **ATOM ATOM** 753 CB LEU A 54151.460 -6.929 3.488 1.00 0.00 C **ATOM** 754 CG LEUA 54151.434 -6.309 2.090 1.00 0.00 C 755 CD1 LEU A 54152.561 -6.869 1.236 1.00 0.00 C **ATOM ATOM** 756 CD2 LEU A 54150.087 -6.552 1.425 1.00 0.00 C 757 H LEUA 54151.852 -4.472 3.997 1.00 0.00 H **ATOM ATOM** 758 HA LEUA 54149.635 -6.202 4.335 1.00 0.00 H 759 1HB LEUA 54152.490 -7.011 3.805 1.00 0.00 H ATOM 760 2HB LEU A 54151.042 -7.922 3.424 1.00 0.00 H **ATOM** 761 HG LEUA 54151.578 -5.241 2.175 1.00 0.00 H **ATOM** 762 1HD1 LEU A 54153.480 -6.863 1.804 1.00 0.00 H **ATOM** ATOM 763 2HD1 LEU A 54152.680 -6.260 0.352 1.00 0.00 H 764 3HD1 LEU A 54152.324 -7.882 0.947 1.00 0.00 H **ATOM** 765 1HD2 LEU A 54149.633 -7.438 1.847 1.00 0.00 H ATOM 766 2HD2 LEU A 54150.229 -6.692 0.364 1.00 0.00 H ATOM 767 3HD2 LEU A 54149.443 -5.702 1.595 1.00 0.00 H **ATOM** 768 N GLUA 55149.958 -7.528 6.413 1.00 0.00 N **ATOM** 769 CA GLUA 55150.067 -8.176 7.715 1.00 0.00 C **ATOM** 770 C GLUA 55151.139 -9.261 7.696 1.00 0.00 C **ATOM** 771 O GLUA 55151.836 -9.478 8.686 1.00 0.00 O **ATOM** ATOM 772 CB GLU A 55148.722 -8.779 8.123 1.00 0.00 C 773 CG GLU A 55147.657 -7.739 8.430 1.00 0.00 C ATOM 774 CD GLU A 55146.711 -7.512 7.268 1.00 0.00 C ATOM 775 OE1 GLU A 55146.763 -6.420 6.663 1.00 0.00 O **ATOM** 776 OE2 GLU A 55145.916 -8.426 6.962 1.00 0.00 O ATOM

777 H GLUA 55149.144 -7.655 5.884 1.00 0.00 H ATOM **ATOM** 778 HA GLUA 55150.347 -7.424 8.437 1.00 0.00 H 779 1HB GLU A 55148.361 -9.404 7.319 1.00 0.00 H ATOM 780 2HB GLU A 55148.864 -9.388 9.003 1.00 0.00 H **ATOM** 781 1HG GLU A 55147.083 -8.069 9.283 1.00 0.00 H ATOM 782 2HG GLU A 55148.143 -6.803 8.667 1.00 0.00 H **ATOM** ATOM 783 N ASPA 56151.263 -9.943 6.561 1.00 0.00 N 784 CA ASP A 56152.251 -11.006 6.412 1.00 0.00 C ATOM **ATOM** 785 C ASPA 56153.446 -10.528 5.596 1.00 0.00 C 786 O ASPA 56153.285 -9.897 4.551 1.00 0.00 O **ATOM** 787 CB ASP A 56151.617 -12.228 5.745 1.00 0.00 C **ATOM** 788 CG ASPA 56151.036 -13.201 6.753 1.00 0.00 C **ATOM ATOM** 789 OD1 ASP A 56149.897 -13.665 6.541 1.00 0.00 O 790 OD2 ASP A 56151.722 -13.498 7.754 1.00 0.00 O ATOM 791 H ASPA 56150.678 -9.724 5.806 1.00 0.00 H **ATOM** 792 HA ASP A 56152.591 -11.281 7.399 1.00 0.00 H ATOM 793 1HB ASP A 56150.825 -11.902 5.089 1.00 0.00 H **ATOM ATOM** 794 2HB ASP A 56152.370 -12.744 5.167 1.00 0.00 H 795 N GLUA 57154.646 -10.834 6.078 1.00 0.00 N **ATOM** 796 CA GLUA 57155.870 -10.436 5.392 1.00 0.00 C **ATOM** 797 C GLUA 57155.928 -11.034 3.991 1.00 0.00 C ATOM 798 O GLUA 57156.352 -12.176 3.810 1.00 0.00 O ATOM 799 CB GLU A 57157.095 -10.872 6.197 1.00 0.00 C **ATOM ATOM** 800 CG GLU A 57157.104 -10.349 7.624 1.00 0.00 C 801 CD GLUA 57156.564 -11.358 8.618 1.00 0.00 C ATOM 802 OE1 GLU A 57156.945 -11.284 9.805 1.00 0.00 O **ATOM** 803 OE2 GLU A 57155.759 -12.221 8.210 1.00 0.00 O ATOM 804 H GLUA 57154.710 -11.339 6.915 1.00 0.00 H ATOM 805 HA GLU A 57155.869 -9.359 5.311 1.00 0.00 H ATOM 806 1HB GLU A 57157.123 -11.951 6.233 1.00 0.00 H **ATOM** ATOM 807 2HB GLU A 57157.985 -10.514 5.700 1.00 0.00 H

808 1HG GLU A 57158.120 -10.105 7.898 1.00 0.00 H **ATOM** 809 2HG GLU A 57156.496 -9.458 7.671 1.00 0.00 H **ATOM** 810 N CYS A 58155.499 -10.256 3.003 1.00 0.00 N **ATOM** ATOM 811 CA CYS A 58155.502 -10.709 1.617 1.00 0.00 C 812 C CYS A 58156.853 -10.442 0.960 1.00 0.00 C **ATOM** 813 O CYS A 58157.328 -9.307 0.933 1.00 0.00 O ATOM 814 CB CYS A 58154.392 -10.013 0.828 1.00 0.00 C ATOM 815 SG CYS A 58154.271 -10.539 -0.897 1.00 0.00 S ATOM 816 H CYS A 58155.173 -9.355 3.210 1.00 0.00 H ATOM 817 HA CYS A 58155.319 -11.773 1.616 1.00 0.00 H ATOM 818 1HB CYS A 58153.443 -10.217 1.300 1.00 0.00 H **ATOM** 819 2HB CYS A 58154.570 -8.947 0.835 1.00 0.00 H ATOM **ATOM** 820 HG CYS A 58154.021 -11.467 -0.907 1.00 0.00 H 821 N ALAA 59157.466 -11.496 0.431 1.00 0.00 N ATOM 822 CA ALA A 59158.762 -11.375 -0.226 1.00 0.00 C **ATOM** 823 C ALAA 59158.686 -10.433 -1.423 1.00 0.00 C ATOM 824 O ALAA 59157.969 -10.698 -2.389 1.00 0.00 O **ATOM** 825 CB ALA A 59159.262 -12.744 -0.661 1.00 0.00 C ATOM 826 H ALAA 59157.037 -12.376 0.483 1.00 0.00 H **ATOM** 827 HA ALA A 59159.463 -10.974 0.491 1.00 0.00 H ATOM 828 1HB ALAA 59160.333 -12.710 -0.800 1.00 0.00 H **ATOM** 829 2HB ALA A 59158.788 -13.021 -1.592 1.00 0.00 H **ATOM** 830 3HB ALA A 59159.020 -13.474 0.097 1.00 0.00 H **ATOM ATOM** 831 N GLY A 60159.428 -9.334 -1.352 1.00 0.00 N 832 CA GLY A 60159.430 -8.369 -2.437 1.00 0.00 C **ATOM** 833 C GLY A 60158.687 -7.096 -2.082 1.00 0.00 C **ATOM** 834 O GLY A 60157.935 -6.561 -2.896 1.00 0.00 O ATOM 835 H GLY A 60159.979 -9.176 -0.558 1.00 0.00 H **ATOM** 836 1HA GLY A 60160.452 -8.119 -2.680 1.00 0.00 H **ATOM** 837 2HA GLY A 60158.963 -8.816 -3.302 1.00 0.00 H **ATOM**

ATOM 838 N CYS A 61158.897 -6.610 -0.863 1.00 0.00 N

- ATOM 839 CA CYS A 61158.240 -5.392 -0.402 1.00 0.00 C
- ATOM 840 C CYS A 61159.222 -4.494 0.343 1.00 0.00 C
- ATOM 841 O CYS A 61160.342 -4.903 0.652 1.00 0.00 O
- ATOM 842 CB CYS A 61157.058 -5.738 0.505 1.00 0.00 C
- ATOM 843 SG CYS A 61155.845 -6.842 -0.254 1.00 0.00 S
- ATOM 844 H CYS A 61159.508 -7.081 -0.258 1.00 0.00 H
- ATOM 845 HA CYS A 61157.875 -4.863 -1.270 1.00 0.00 H
- ATOM 846 1HB CYS A 61157.427 -6.219 1.397 1.00 0.00 H
- ATOM 847 2HB CYS A 61156.547 -4.826 0.779 1.00 0.00 H
- ATOM 848 HG CYS A 61154.969 -6.511 -0.042 1.00 0.00 H
- ATOM 849 N THR A 62158.796 -3.268 0.629 1.00 0.00 N
- ATOM 850 CA THR A 62159.637 -2.311 1.338 1.00 0.00 C
- ATOM 851 C THR A 62159.197 -2.171 2.790 1.00 0.00 C
- ATOM 852 O THR A 62158.253 -2.829 3.230 1.00 0.00 O
- ATOM 853 CB THR A 62159.591 -0.949 0.645 1.00 0.00 C
- ATOM 854 OG1 THR A 62158.350 -0.308 0.879 1.00 0.00 O
- ATOM 855 CG2 THR A 62159.791 -1.031 -0.853 1.00 0.00 C
- ATOM 856 H THR A 62157.894 -3.000 0.357 1.00 0.00 H
- ATOM 857 HA THR A 62160.651 -2.682 1.316 1.00 0.00 H
- ATOM 858 HB THR A 62160.376 -0.325 1.050 1.00 0.00 H
- ATOM 859 HG1 THR A 62157.639 -0.850 0.529 1.00 0.00 H
- ATOM 860 1HG2 THR A 62158.928 -1.498 -1.305 1.00 0.00 H
- ATOM 861 2HG2 THR A 62160.671 -1.618 -1.067 1.00 0.00 H
- ATOM 862 3HG2 THR A 62159.913 -0.036 -1.254 1.00 0.00 H
- ATOM 863 N ASPA 63159.886 -1.310 3.533 1.00 0.00 N
- ATOM 864 CA ASP A 63159.564 -1.083 4.937 1.00 0.00 C
- ATOM 865 C ASPA 63158.915 0.283 5.133 1.00 0.00 C
- ATOM 866 O ASPA 63159.079 0.916 6.177 1.00 0.00 O
- ATOM 867 CB ASPA 63160.827 -1.189 5.794 1.00 0.00 C
- ATOM 868 CG ASPA 63161.869 -0.155 5.418 1.00 0.00 C
- ATOM 869 OD1 ASP A 63162.279 0.624 6.304 1.00 0.00 O

870 OD2 ASP A 63162.277 -0.124 4.237 1.00 0.00 O **ATOM ATOM** 871 H ASPA 63160.627 -0.815 3.126 1.00 0.00 H 872 HA ASPA 63158.866 -1.847 5.245 1.00 0.00 H **ATOM ATOM** 873 1HB ASPA 63160.564 -1.046 6.832 1.00 0.00 H **ATOM** 874 2HB ASPA 63161.258 -2.171 5.668 1.00 0.00 H **ATOM** 875 N GLY A 64158.180 0.734 4.122 1.00 0.00 N 876 CA GLY A 64157.517 2.023 4.204 1.00 0.00 C ATOM **ATOM** 877 C GLYA 64158.203 3.081 3.362 1.00 0.00 C ATOM 878 O GLY A 64158.146 4.269 3.680 1.00 0.00 O 879 H GLY A 64158.085 0.187 3.315 1.00 0.00 H ATOM ATOM 880 1HA GLY A 64156.498 1.913 3.865 1.00 0.00 H 881 2HA GLY A 64157.511 2.347 5.233 1.00 0.00 H ATOM **ATOM** 882 N THR A 65158.852 2.650 2.285 1.00 0.00 N 883 CA THR A 65159.552 3.569 1.395 1.00 0.00 C ATOM **ATOM** 884 C THR A 65159.130 3.350 -0.054 1.00 0.00 C 885 O THR A 65159.318 2.267 -0.609 1.00 0.00 O ATOM 886 CB THR A 65161.065 3.392 1.530 1.00 0.00 C **ATOM** ATOM 887 OG1 THR A 65161.396 2.023 1.693 1.00 0.00 O **ATOM** 888 CG2 THR A 65161.654 4.148 2.700 1.00 0.00 C 889 H THR A 65158.861 1.690 2.085 1.00 0.00 H ATOM

890 HA THR A 65159.290 4.576 1.685 1.00 0.00 H ATOM 891 HB THR A 65161.541 3.751 0.629 1.00 0.00 H **ATOM** 892 HG1 THR A 65161.415 1.594 0.834 1.00 0.00 H **ATOM ATOM** 893 1HG2 THR A 65160.857 4.539 3.315 1.00 0.00 H 894 2HG2 THR A 65162.259 4.965 2.333 1.00 0.00 H **ATOM** 895 3HG2 THR A 65162.268 3.482 3.288 1.00 0.00 H **ATOM** 896 N PHE A 66158.560 4.385 -0.663 1.00 0.00 N **ATOM** 897 CA PHE A 66158.112 4.304 -2.048 1.00 0.00 C ATOM **ATOM** 898 C PHE A 66159.029 5.108 -2.965 1.00 0.00 C 899 O PHE A 66159.115 6.331 -2.857 1.00 0.00 O **ATOM** 900 CB PHE A 66156.675 4.814 -2.172 1.00 0.00 C ATOM

ATOM 901 CG PHE A 66156.029 4.474 -3.484 1.00 0.00 C 902 CD1 PHE A 66155.625 5.475 -4.354 1.00 0.00 C ATOM 903 CD2 PHE A 66155.826 3.153 -3.849 1.00 0.00 C ATOM 904 CE1 PHE A 66155.032 5.165 -5.562 1.00 0.00 C ATOM ATOM 905 CE2 PHE A 66155.232 2.836 -5.057 1.00 0.00 C ATOM 906 CZ PHE A 66154.834 3.843 -5.914 1.00 0.00 C 907 H PHE A 66158.438 5.222 -0.168 1.00 0.00 H ATOM 908 HA PHE A 66158.143 3.268 -2.347 1.00 0.00 H ATOM 909 1HB PHE A 66156.077 4.380 -1.385 1.00 0.00 H ATOM ATOM 910 2HB PHE A 66156.672 5.890 -2.068 1.00 0.00 H 911 HD1 PHE A 66155.780 6.509 -4.080 1.00 0.00 H ATOM 912 HD2 PHE A 66156.137 2.364 -3.179 1.00 0.00 H ATOM 913 HE1 PHE A 66154.721 5.954 -6.231 1.00 0.00 H **ATOM** 914 HE2 PHE A 66155.080 1.803 -5.329 1.00 0.00 H ATOM 915 HZ PHE A 66154.371 3.598 -6.858 1.00 0.00 H ATOM **ATOM** 916 N ARGA 67159.713 4.411 -3.867 1.00 0.00 N 917 CA ARG A 67160.624 5.059 -4.803 1.00 0.00 C **ATOM** 918 C ARGA 67161.735 5.794 -4.062 1.00 0.00 C **ATOM** 919 O ARGA 67162.174 6.864 -4.482 1.00 0.00 O **ATOM** 920 CB ARG A 67159.858 6.036 -5.698 1.00 0.00 C **ATOM ATOM** 921 CG ARG A 67158.819 5.365 -6.581 1.00 0.00 C 922 CD ARG A 67158.307 6.310 -7.654 1.00 0.00 C **ATOM** 923 NE ARG A 67159.178 6.330 -8.827 1.00 0.00 N **ATOM** 924 CZ ARG A 67159.307 5.310 -9.672 1.00 0.00 C **ATOM** 925 NH1 ARG A 67158.624 4.189 -9.480 1.00 0.00 N **ATOM** 926 NH2 ARG A 67160.122 5.412 -10.714 1.00 0.00 N ATOM 927 H ARG A 67159.602 3.438 -3.904 1.00 0.00 H ATOM 928 HA ARG A 67161.066 4.291 -5.420 1.00 0.00 H ATOM 929 1HB ARG A 67159.357 6.759 -5.074 1.00 0.00 H **ATOM** 930 2HB ARG A 67160.564 6.549 -6.336 1.00 0.00 H **ATOM** 931 1HG ARG A 67159.266 4.504 -7.056 1.00 0.00 H

- ATOM 932 2HG ARG A 67157.989 5.048 -5.965 1.00 0.00 H
- ATOM 933 1HD ARG A 67157.321 5.990 -7.957 1.00 0.00 H
- ATOM 934 2HD ARG A 67158.250 7.306 -7.242 1.00 0.00 H
- ATOM 935 HE ARG A 67159.695 7.147 -8.993 1.00 0.00 H
- ATOM 936 1HH1 ARG A 67158.008 4.106 -8.697 1.00 0.00 H
- ATOM 937 2HH1 ARG A 67158.725 3.426 -10.119 1.00 0.00 H
- ATOM 938 1HH2 ARG A 67160.639 6.254 -10.864 1.00 0.00 H
- ATOM 939 2HH2 ARG A 67160.219 4.646 -11.348 1.00 0.00 H
- ATOM 940 N GLY A 68162.187 5.212 -2.955 1.00 0.00 N
- ATOM 941 CA GLY A 68163.243 5.827 -2.173 1.00 0.00 C
- ATOM 942 C GLY A 68162.762 7.037 -1.396 1.00 0.00 C
- ATOM 943 O GLY A 68163.536 7.953 -1.119 1.00 0.00 O
- ATOM 944 H GLY A 68161.800 4.359 -2.667 1.00 0.00 H
- ATOM 945 1HA GLY A 68163.632 5.098 -1.478 1.00 0.00 H
- ATOM 946 2HA GLY A 68164.037 6.132 -2.838 1.00 0.00 H
- ATOM 947 N THR A 69161.481 7.040 -1.044 1.00 0.00 N
- ATOM 948 CA THR A 69160.897 8.147 -0.295 1.00 0.00 C
- ATOM 949 C THR A 69160.046 7.632 0.861 1.00 0.00 C
- ATOM 950 O THR A 69158.867 7.323 0.687 1.00 0.00 O
- ATOM 951 CB THR A 69160.049 9.023 -1.217 1.00 0.00 C
- ATOM 952 OG1 THR A 69160.737 9.293 -2.425 1.00 0.00 O
- ATOM 953 CG2 THR A 69159.669 10.351 -0.598 1.00 0.00 C
- ATOM 954 H THR A 69160.914 6.280 -1.294 1.00 0.00 H
- ATOM 955 HA THR A 69161.706 8.738 0.105 1.00 0.00 H
- ATOM 956 HB THR A 69159.135 8.498 -1.457 1.00 0.00 H
- ATOM 957 HG1 THR A 69161.578 9.711 -2.228 1.00 0.00 H
- ATOM 958 1HG2 THR A 69160.045 11.156 -1.213 1.00 0.00 H
- ATOM 959 2HG2 THR A 69160.099 10.423 0.390 1.00 0.00 H
- ATOM 960 3HG2 THR A 69158.594 10.423 -0.530 1.00 0.00 H
- ATOM 961 N ARG A 70160.651 7.542 2.041 1.00 0.00 N
- ATOM 962 CA ARG A 70159.949 7.064 3.226 1.00 0.00 C

963 C ARGA 70158.808 8.005 3.600 1.00 0.00 C ATOM 964 O ARG A 70158.979 9.224 3.623 1.00 0.00 O **ATOM** 965 CB ARG A 70160.920 6.931 4.401 1.00 0.00 C ATOM 966 CG ARG A 70160.340 6.178 5.588 1.00 0.00 C **ATOM** 967 CD ARG A 70160.741 6.817 6.909 1.00 0.00 C **ATOM** 968 NE ARG A 70161.752 6.032 7.613 1.00 0.00 N ATOM ATOM 969 CZ ARG A 70163.055 6.085 7.344 1.00 0.00 C 970 NH1 ARG A 70163.511 6.883 6.385 1.00 0.00 N **ATOM** 971 NH2 ARG A 70163.905 5.337 8.033 1.00 0.00 N **ATOM** 972 H ARG A 70161.592 7.802 2.115 1.00 0.00 H **ATOM** 973 HA ARGA 70159.538 6.091 2.999 1.00 0.00 H **ATOM ATOM** 974 1HB ARG A 70161.803 6.407 4.066 1.00 0.00 H 975 2HB ARG A 70161.203 7.920 4.732 1.00 0.00 H **ATOM** 976 1HG ARG A 70159.263 6.180 5.511 1.00 0.00 H **ATOM** 977 2HG ARG A 70160.703 5.159 5.566 1.00 0.00 H **ATOM** 978 1HD ARG A 70161.136 7.802 6.714 1.00 0.00 H ATOM 979 2HD ARG A 70159.863 6.899 7.533 1.00 0.00 H **ATOM** 980 HE ARG A 70161.444 5.432 8.325 1.00 0.00 H **ATOM** 981 1HH1 ARG A 70162.877 7.450 5.861 1.00 0.00 H ATOM 982 2HH1 ARG A 70164.491 6.919 6.190 1.00 0.00 H **ATOM** 983 1HH2 ARG A 70163.567 4.734 8.756 1.00 0.00 H ATOM 984 2HH2 ARG A 70164.884 5.377 7.832 1.00 0.00 H **ATOM** 985 N TYR A 71157.646 7.431 3.890 1.00 0.00 N **ATOM** 986 CA TYR A 71156.476 8.218 4.264 1.00 0.00 C **ATOM** 987 C TYR A 71156.055 7.920 5.700 1.00 0.00 C **ATOM** 988 O TYR A 71155.648 8.817 6.437 1.00 0.00 O **ATOM** 989 CB TYR A 71155.316 7.932 3.309 1.00 0.00 C **ATOM** 990 CG TYR A 71155.479 8.569 1.948 1.00 0.00 C **ATOM** 991 CD1 TYR A 71155.397 7.809 0.788 1.00 0.00 C **ATOM** 992 CD2 TYR A 71155.717 9.933 1.823 1.00 0.00 C **ATOM** 993 CE1 TYR A 71155.547 8.389 -0.457 1.00 0.00 C ATOM

994 CE2 TYR A 71155.867 10.520 0.581 1.00 0.00 C ATOM 995 CZ TYR A 71155.781 9.745 -0.555 1.00 0.00 C 996 OH TYR A 71155.931 10.325 -1.793 1.00 0.00 O ATOM 997 H TYR A 71157.572 6.454 3.855 1.00 0.00 H ATOM 998 HA TYR A 71156.742 9.262 4.190 1.00 0.00 H ATOM 999 1HB TYR A 71155.232 6.864 3.166 1.00 0.00 H ATOM ATOM 1000 2HB TYR A 71154.401 8.305 3.744 1.00 0.00 H ATOM 1001 HD1 TYR A 71155.213 6.748 0.869 1.00 0.00 H ATOM 1002 HD2 TYR A 71155.785 10.538 2.716 1.00 0.00 H ATOM 1003 HE1 TYR A 71155.480 7.781 -1.347 1.00 0.00 H ATOM 1004 HE2 TYR A 71156.051 11.581 0.506 1.00 0.00 H ATOM 1005 HH TYR A 71155.460 11.161 -1.814 1.00 0.00 H ATOM 1006 N PHE A 72156.155 6.653 6.089 1.00 0.00 N ATOM 1007 CA PHE A 72155.784 6.235 7.436 1.00 0.00 C ATOM 1008 C PHE A 72156.783 5.220 7.984 1.00 0.00 C ATOM 1009 O PHE A 72157.758 4.872 7.320 1.00 0.00 O ATOM 1010 CB PHE A 72154.378 5.635 7.437 1.00 0.00 C ATOM 1011 CG PHE A 72154.144 4.648 6.328 1.00 0.00 C ATOM 1012 CD1 PHE A 72153.812 5.083 5.055 1.00 0.00 C ATOM 1013 CD2 PHE A 72154.258 3.287 6.559 1.00 0.00 C ATOM 1014 CE1 PHE A 72153.598 4.179 4.033 1.00 0.00 C ATOM 1015 CE2 PHE A 72154.045 2.378 5.541 1.00 0.00 C ATOM 1016 CZ PHE A 72153.714 2.824 4.276 1.00 0.00 C ATOM 1017 H PHE A 72156.486 5.982 5.455 1.00 0.00 H ATOM 1018 HA PHE A 72155.795 7.110 8.068 1.00 0.00 H ATOM 1019 1HB PHE A 72154.212 5.125 8.375 1.00 0.00 H ATOM 1020 2HB PHE A 72153.654 6.431 7.333 1.00 0.00 H ATOM 1021 HD1 PHE A 72153.721 6.142 4.864 1.00 0.00 H ATOM 1022 HD2 PHE A 72154.517 2.937 7.548 1.00 0.00 H ATOM 1023 HE1 PHE A 72153.338 4.530 3.045 1.00 0.00 H ATOM 1024 HE2 PHE A 72154.137 1.319 5.734 1.00 0.00 H

ATOM 1025 HZ PHE A 72153.547 2.115 3.479 1.00 0.00 H ATOM 1026 N THR A 73156.533 4.750 9.202 1.00 0.00 N ATOM 1027 CA THR A 73157.409 3.775 9.840 1.00 0.00 C ATOM 1028 C THR A 73156.665 2.470 10.108 1.00 0.00 C ATOM 1029 O THR A 73155.816 2.398 10.997 1.00 0.00 O ATOM 1030 CB THR A 73157.964 4.337 11.151 1.00 0.00 C ATOM 1031 OG1 THR A 73157.040 5.231 11.743 1.00 0.00 O ATOM 1032 CG2 THR A 73159.273 5.077 10.977 1.00 0.00 C ATOM 1033 H THR A 73155.738 5.066 9.682 1.00 0.00 H ATOM 1034 HA THR A 73158.230 3.576 9.168 1.00 0.00 H ATOM 1035 HB THR A 73158.133 3.520 11.837 1.00 0.00 H ATOM 1036 HG1 THR A 73157.405 5.572 12.564 1.00 0.00 H ATOM 1037 1HG2 THR A 73159.290 5.554 10.008 1.00 0.00 H ATOM 1038 2HG2 THR A 73160.093 4.377 11.048 1.00 0.00 H ATOM 1039 3HG2 THR A 73159.369 5.824 11.749 1.00 0.00 H ATOM 1040 N CYS A 74156.991 1.440 9.335 1.00 0.00 N ATOM 1041 CA CYS A 74156.354 0.138 9.488 1.00 0.00 C ATOM 1042 C CYS A 74157.390 -0.982 9.465 1.00 0.00 C ATOM 1043 O CYS A 74158.591 -0.728 9.368 1.00 0.00 O ATOM 1044 CB CYS A 74155.323 -0.083 8.379 1.00 0.00 C ATOM 1045 SG CYS A 74153.706 0.652 8.718 1.00 0.00 S ATOM 1046 H CYS A 74157.676 1.559 8.643 1.00 0.00 H ATOM 1047 HA CYS A 74155.850 0.125 10.442 1.00 0.00 H ATOM 1048 1HB CYS A 74155.694 0.350 7.462 1.00 0.00 H ATOM 1049 2HB CYS A 74155.180 -1.144 8.237 1.00 0.00 H ATOM 1050 HG CYS A 74153.749 1.078 9.577 1.00 0.00 H ATOM 1051 N ALAA 75156.918 -2.220 9.553 1.00 0.00 N ATOM 1052 CA ALA A 75157.803 -3.378 9.542 1.00 0.00 C ATOM 1053 C ALAA 75158.397 -3.602 8.156 1.00 0.00 C ATOM 1054 O ALAA 75157.882 -3.095 7.160 1.00 0.00 O ATOM 1055 CB ALA A 75157.053 -4.619 10.004 1.00 0.00 C

ATOM 1056 H ALAA 75155.951 -2.359 9.628 1.00 0.00 H ATOM 1057 HA ALA A 75158.605 -3.190 10.241 1.00 0.00 H ATOM 1058 1HB ALA A 75157.153 -4.723 11.074 1.00 0.00 H ATOM 1059 2HB ALA A 75157.466 -5.490 9.518 1.00 0.00 H ATOM 1060 3HB ALA A 75156.008 -4.525 9.747 1.00 0.00 H ATOM 1061 N LEUA 76159.484 -4.366 8.100 1.00 0.00 N ATOM 1062 CA LEU A 76160.148 -4.658 6.836 1.00 0.00 C ATOM 1063 C LEUA 76159.378 -5.712 6.046 1.00 0.00 C ATOM 1064 O LEUA 76158.795 -6.631 6.623 1.00 0.00 O ATOM 1065 CB LEU A 76161.579 -5.137 7.087 1.00 0.00 C ATOM 1066 CG LEU A 76162.627 -4.025 7.176 1.00 0.00 C ATOM 1067 CD1 LEU A 76163.728 -4.406 8.153 1.00 0.00 C ATOM 1068 CD2 LEU A 76163.208 -3.731 5.802 1.00 0.00 C ATOM 1069 H LEU A 76159.846 -4.742 8.929 1.00 0.00 H ATOM 1070 HA LEU A 76160.179 -3.745 6.259 1.00 0.00 H ATOM 1071 1HB LEU A 76161.593 -5.692 8.013 1.00 0.00 H ATOM 1072 2HB LEU A 76161.861 -5.800 6.284 1.00 0.00 H ATOM 1073 HG LEU A 76162.155 -3.124 7.541 1.00 0.00 H ATOM 1074 1HD1 LEU A 76164.661 -3.965 7.834 1.00 0.00 H ATOM 1075 2HD1 LEU A 76163.828 -5.481 8.180 1.00 0.00 H ATOM 1076 3HD1 LEU A 76163.476 -4.044 9.139 1.00 0.00 H ATOM 1077 1HD2 LEU A 76164.135 -4.272 5.681 1.00 0.00 H ATOM 1078 2HD2 LEU A 76163.395 -2.671 5.708 1.00 0.00 H ATOM 1079 3HD2 LEU A 76162.508 -4.041 5.040 1.00 0.00 H ATOM 1080 N LYS A 77159.379 -5.572 4.724 1.00 0.00 N ATOM 1081 CA LYS A 77158.681 -6.513 3.857 1.00 0.00 C ATOM 1082 C LYS A 77157.188 -6.536 4.170 1.00 0.00 C ATOM 1083 O LYS A 77156.545 -7.584 4.103 1.00 0.00 O ATOM 1084 CB LYS A 77159.268 -7.917 4.011 1.00 0.00 C ATOM 1085 CG LYS A 77160.742 -8.002 3.648 1.00 0.00 C ATOM 1086 CD LYS A 77160.936 -8.190 2.152 1.00 0.00 C

ATOM 1087 CE LYS A 77162.179 -7.470 1.656 1.00 0.00 C ATOM 1088 NZ LYS A 77162.702 -8.067 0.396 1.00 0.00 N ATOM 1089 H LYS A 77159.861 -4.819 4.324 1.00 0.00 H ATOM 1090 HA LYS A 77158.816 -6.185 2.837 1.00 0.00 H ATOM 1091 1HB LYS A 77159.154 -8.231 5.038 1.00 0.00 H ATOM 1092 2HB LYS A 77158.722 -8.595 3.373 1.00 0.00 H ATOM 1093 1HG LYS A 77161.232 -7.089 3.952 1.00 0.00 H ATOM 1094 2HG LYS A 77161.183 -8.840 4.168 1.00 0.00 H ATOM 1095 1HD LYS A 77161.036 -9.245 1.942 1.00 0.00 H ATOM 1096 2HD LYS A 77160.073 -7.799 1.634 1.00 0.00 H ATOM 1097 1HE LYS A 77161.932 -6.434 1.478 1.00 0.00 H ATOM 1098 2HE LYS A 77162.943 -7.531 2.418 1.00 0.00 H ATOM 1099 1HZ LYS A 77162.608 -9.102 0.425 1.00 0.00 H ATOM 1100 2HZ LYS A 77163.706 -7.824 0.274 1.00 0.00 H ATOM 1101 3HZ LYS A 77162.168 -7.703 -0.419 1.00 0.00 H ATOM 1102 N LYS A 78156.643 -5.373 4.513 1.00 0.00 N ATOM 1103 CA LYS A 78155.224 -5.259 4.837 1.00 0.00 C ATOM 1104 C LYS A 78154.686 -3.886 4.449 1.00 0.00 C ATOM 1105 O LYS A 78153.863 -3.308 5.158 1.00 0.00 O ATOM 1106 CB LYS A 78155.000 -5.505 6.330 1.00 0.00 C ATOM 1107 CG LYS A 78155.513 -6.854 6.809 1.00 0.00 C ATOM 1108 CD LYS A 78155.303 -7.030 8.304 1.00 0.00 C ATOM 1109 CE LYS A 78154.065 -7.862 8.598 1.00 0.00 C ATOM 1110 NZ LYS A 78153.334 -7.367 9.797 1.00 0.00 N ATOM 1111 H LYS A 78157.206 -4.572 4.548 1.00 0.00 H ATOM 1112 HA LYS A 78154.695 -6.012 4.274 1.00 0.00 H ATOM 1113 1HB LYS A 78155.507 -4.732 6.890 1.00 0.00 H ATOM 1114 2HB LYS A 78153.942 -5.453 6.537 1.00 0.00 H ATOM 1115 1HG LYS A 78154.984 -7.636 6.285 1.00 0.00 H ATOM 1116 2HG LYS A 78156.570 -6.924 6.592 1.00 0.00 H ATOM 1117 1HD LYS A 78156.165 -7.526 8.723 1.00 0.00 H ATOM 1118 2HD LYS A 78155.188 -6.057 8.759 1.00 0.00 H ATOM 1119 1HE LYS A 78153.407 -7.820 7.743 1.00 0.00 H ATOM 1120 2HE LYS A 78154.367 -8.886 8.768 1.00 0.00 H ATOM 1121 1HZ LYS A 78152.990 -6.399 9.630 1.00 0.00 H ATOM 1122 2HZ LYS A 78153.965 -7.361 10.623 1.00 0.00 H ATOM 1123 3HZ LYS A 78152.521 -7.982 9.999 1.00 0.00 H ATOM 1124 N ALAA 79155.156 -3.369 3.318 1.00 0.00 N ATOM 1125 CA ALA A 79154.722 -2.064 2.836 1.00 0.00 C ATOM 1126 C ALAA 79154.543 -2.070 1.322 1.00 0.00 C ATOM 1127 O ALAA 79155.517 -1.992 0.571 1.00 0.00 O ATOM 1128 CB ALA A 79155.720 -0.992 3.247 1.00 0.00 C ATOM 1129 H ALAA 79155.811 -3.879 2.796 1.00 0.00 H ATOM 1130 HA ALAA 79153.774 -1.837 3.299 1.00 0.00 H ATOM 1131 1HB ALAA 79155.219 -0.036 3.300 1.00 0.00 H ATOM 1132 2HB ALAA 79156.515 -0.941 2.518 1.00 0.00 H ATOM 1133 3HB ALA A 79156.133 -1.237 4.214 1.00 0.00 H ATOM 1134 N LEUA 80153.294 -2.162 0.878 1.00 0.00 N ATOM 1135 CA LEU A 80152.988 -2.178 -0.548 1.00 0.00 C ATOM 1136 C LEU A 80152.143 -0.968 -0.936 1.00 0.00 C ATOM 1137 O LEUA 80150.992 -0.842 -0.519 1.00 0.00 O ATOM 1138 CB LEU A 80152.252 -3.467 -0.919 1.00 0.00 C ATOM 1139 CG LEU A 80151.835 -3.574 -2.387 1.00 0.00 C ATOM 1140 CD1 LEU A 80153.048 -3.819 -3.270 1.00 0.00 C ATOM 1141 CD2 LEU A 80150.809 -4.683 -2.568 1.00 0.00 C ATOM 1142 H LEUA 80152.561 -2.220 1.525 1.00 0.00 H ATOM 1143 HA LEU A 80153.922 -2.138 -1.088 1.00 0.00 H ATOM 1144 1HB LEU A 80152.896 -4.303 -0.687 1.00 0.00 H ATOM 1145 2HB LEU A 80151.364 -3.538 -0.309 1.00 0.00 H ATOM 1146 HG LEU A 80151.381 -2.644 -2.693 1.00 0.00 H ATOM 1147 1HD1 LEU A 80153.457 -2.872 -3.590 1.00 0.00 H ATOM 1148 2HD1 LEU A 80152.753 -4.394 -4.136 1.00 0.00 H ATOM 1149 3HD1 LEU A 80153.796 -4.364 -2.713 1.00 0.00 H ATOM 1150 1HD2 LEU A 80150.935 -5.134 -3.541 1.00 0.00 H ATOM 1151 2HD2 LEU A 80149.814 -4.270 -2.488 1.00 0.00 H ATOM 1152 3HD2 LEU A 80150.950 -5.432 -1.803 1.00 0.00 H ATOM 1153 N PHE A 81152.723 -0.082 -1.739 1.00 0.00 N ATOM 1154 CA PHE A 81152.024 1.117 -2.185 1.00 0.00 C ATOM 1155 C PHE A 81151.158 0.819 -3.405 1.00 0.00 C ATOM 1156 O PHE A 81151.569 0.089 -4.307 1.00 0.00 O ATOM 1157 CB PHE A 81153.027 2.224 -2.515 1.00 0.00 C ATOM 1158 CG PHE A 81153.688 2.816 -1.303 1.00 0.00 C ATOM 1159 CD1 PHE A 81153.308 4.060 -0.828 1.00 0.00 C ATOM 1160 CD2 PHE A 81154.690 2.126 -0.639 1.00 0.00 C ATOM 1161 CE1 PHE A 81153.915 4.607 0.287 1.00 0.00 C ATOM 1162 CE2 PHE A 81155.300 2.668 0.477 1.00 0.00 C ATOM 1163 CZ PHE A 81154.912 3.909 0.941 1.00 0.00 C ATOM 1164 H PHE A 81153.643 -0.239 -2.039 1.00 0.00 H ATOM 1165 HA PHE A 81151.388 1.449 -1.379 1.00 0.00 H ATOM 1166 1HB PHE A 81153.800 1.822 -3.151 1.00 0.00 H ATOM 1167 2HB PHE A 81152.515 3.020 -3.037 1.00 0.00 H ATOM 1168 HD1 PHE A 81152.527 4.606 -1.338 1.00 0.00 H ATOM 1169 HD2 PHE A 81154.995 1.156 -1.000 1.00 0.00 H ATOM 1170 HE1 PHE A 81153.609 5.579 0.647 1.00 0.00 H ATOM 1171 HE2 PHE A 81156.080 2.121 0.985 1.00 0.00 H ATOM 1172 HZ PHE A 81155.388 4.335 1.812 1.00 0.00 H ATOM 1173 N VALA 82149.959 1.389 -3.427 1.00 0.00 N ATOM 1174 CA VALA 82149.035 1.184 -4.535 1.00 0.00 C ATOM 1175 C VALA 82148.156 2.412 -4.753 1.00 0.00 C ATOM 1176 O VALA 82148.101 3.306 -3.909 1.00 0.00 O ATOM 1177 CB VALA 82148.134 -0.041 -4.297 1.00 0.00 C ATOM 1178 CG1 VAL A 82148.953 -1.322 -4.333 1.00 0.00 C ATOM 1179 CG2 VAL A 82147.392 0.090 -2.976 1.00 0.00 C

ATOM 1180 H VALA 82149.687 1.962 -2.677 1.00 0.00 H ATOM 1181 HA VALA 82149.619 1.009 -5.427 1.00 0.00 H ATOM 1182 HB VALA 82147.404 -0.087 -5.093 1.00 0.00 H ATOM 1183 1HG1 VAL A 82148.303 -2.170 -4.174 1.00 0.00 H ATOM 1184 2HG1 VAL A 82149.702 -1.292 -3.555 1.00 0.00 H ATOM 1185 3HG1 VAL A 82149.436 -1.415 -5.295 1.00 0.00 H ATOM 1186 1HG2 VAL A 82147.988 -0.338 -2.185 1.00 0.00 H ATOM 1187 2HG2 VAL A 82146.449 -0.432 -3.039 1.00 0.00 H ATOM 1188 3HG2 VAL A 82147.212 1.134 -2.767 1.00 0.00 H ATOM 1189 N LYS A 83147.471 2.448 -5.891 1.00 0.00 N ATOM 1190 CA LYS A 83146.594 3.565 -6.221 1.00 0.00 C ATOM 1191 C LYS A 83145.381 3.596 -5.299 1.00 0.00 C ATOM 1192 O LYS A 83144.624 2.629 -5.217 1.00 0.00 O ATOM 1193 CB LYS A 83146.139 3.470 -7.679 1.00 0.00 C ATOM 1194 CG LYS A 83147.278 3.584 -8.680 1.00 0.00 C ATOM 1195 CD LYS A 83146.839 3.163 -10.073 1.00 0.00 C ATOM 1196 CE LYS A 83147.457 4.048 -11.143 1.00 0.00 C ATOM 1197 NZ LYS A 83147.818 3.274 -12.363 1.00 0.00 N ATOM 1198 H LYS A 83147.557 1.704 -6.524 1.00 0.00 H ATOM 1199 HA LYS A 83147.155 4.478 -6.087 1.00 0.00 H ATOM 1200 1HB LYS A 83145.649 2.520 -7.830 1.00 0.00 H ATOM 1201 2HB LYS A 83145.434 4.265 -7.876 1.00 0.00 H ATOM 1202 1HG LYS A 83147.612 4.610 -8.714 1.00 0.00 H ATOM 1203 2HG LYS A 83148.090 2.948 -8.359 1.00 0.00 H ATOM 1204 1HD LYS A 83147.145 2.142 -10.243 1.00 0.00 H ATOM 1205 2HD LYS A 83145.763 3.233 -10.137 1.00 0.00 H ATOM 1206 1HE LYS A 83146.748 4.815 -11.411 1.00 0.00 H ATOM 1207 2HE LYS A 83148.348 4.506 -10.741 1.00 0.00 H ATOM 1208 1HZ LYS A 83148.624 3.721 -12.844 1.00 0.00 H ATOM 1209 2HZ LYS A 83147.011 3.243 -13.018 1.00 0.00 H ATOM 1210 3HZ LYS A 83148.078 2.300 -12.105 1.00 0.00 H

ATOM 1211 N LEU A 84145.203 4.715 -4.606 1.00 0.00 N ATOM 1212 CA LEU A 84144.082 4.880 -3.689 1.00 0.00 C ATOM 1213 C LEU A 84142.752 4.717 -4.418 1.00 0.00 C ATOM 1214 O LEU A 84141.808 4.136 -3.885 1.00 0.00 O ATOM 1215 CB LEU A 84144.149 6.254 -3.018 1.00 0.00 C ATOM 1216 CG LEU A 84142.966 6.592 -2.109 1.00 0.00 C ATOM 1217 CD1 LEU A 84143.161 5.981 -0.730 1.00 0.00 C ATOM 1218 CD2 LEU A 84142.791 8.100 -2.004 1.00 0.00 C ATOM 1219 H LEU A 84145.841 5.450 -4.716 1.00 0.00 H ATOM 1220 HA LEU A 84144.160 4.115 -2.931 1.00 0.00 H ATOM 1221 1HB LEU A 84145.054 6.300 -2.429 1.00 0.00 H ATOM 1222 2HB LEU A 84144.206 7.004 -3.793 1.00 0.00 H ATOM 1223 HG LEU A 84142.063 6.179 -2.533 1.00 0.00 H ATOM 1224 1HD1 LEU A 84142.445 6.406 -0.043 1.00 0.00 H ATOM 1225 2HD1 LEU A 84144.162 6.188 -0.382 1.00 0.00 H ATOM 1226 3HD1 LEU A 84143.014 4.912 -0.787 1.00 0.00 H ATOM 1227 1HD2 LEU A 84142.772 8.530 -2.995 1.00 0.00 H ATOM 1228 2HD2 LEU A 84143.614 8.521 -1.445 1.00 0.00 H ATOM 1229 3HD2 LEU A 84141.863 8.321 -1.498 1.00 0.00 H ATOM 1230 N LYS A 85142.688 5.234 -5.641 1.00 0.00 N ATOM 1231 CA LYS A 85141.474 5.146 -6.444 1.00 0.00 C ATOM 1232 C LYS A 85141.139 3.693 -6.773 1.00 0.00 C ATOM 1233 O LYS A 85139.984 3.356 -7.028 1.00 0.00 O ATOM 1234 CB LYS A 85141.633 5.950 -7.735 1.00 0.00 C ATOM 1235 CG LYS A 85142.797 5.492 -8.599 1.00 0.00 C ATOM 1236 CD LYS A 85143.178 6.548 -9.624 1.00 0.00 C ATOM 1237 CE LYS A 85144.685 6.620 -9.814 1.00 0.00 C ATOM 1238 NZ LYS A 85145.077 7.728 -10.729 1.00 0.00 N ATOM 1239 H LYS A 85143.474 5.685 -6.012 1.00 0.00 H ATOM 1240 HA LYS A 85140.664 5.566 -5.867 1.00 0.00 H ATOM 1241 1HB LYS A 85140.726 5.860 -8.316 1.00 0.00 H

ATOM 1242 2HB LYS A 85141.786 6.989 -7.483 1.00 0.00 H ATOM 1243 1HG LYS A 85143.648 5.297 -7.964 1.00 0.00 H ATOM 1244 2HG LYS A 85142.515 4.586 -9.115 1.00 0.00 H ATOM 1245 1HD LYS A 85142.718 6.301 -10.569 1.00 0.00 H ATOM 1246 2HD LYS A 85142.820 7.509 -9.287 1.00 0.00 H ATOM 1247 1HE LYS A 85145.149 6.779 -8.852 1.00 0.00 H ATOM 1248 2HE LYS A 85145.028 5.683 -10.228 1.00 0.00 H ATOM 1249 1HZ LYS A 85146.064 8.004 -10.553 1.00 0.00 H ATOM 1250 2HZ LYS A 85144.465 8.553 -10.574 1.00 0.00 H ATOM 1251 3HZ LYS A 85144.984 7.423 -11.719 1.00 0.00 H ATOM 1252 N SER A 86142.158 2.837 -6.765 1.00 0.00 N ATOM 1253 CA SER A 86141.968 1.423 -7.064 1.00 0.00 C ATOM 1254 C SER A 86141.945 0.594 -5.782 1.00 0.00 C ATOM 1255 O SER A 86142.403 -0.548 -5.762 1.00 0.00 O ATOM 1256 CB SER A 86143,077 0.922 -7.990 1.00 0.00 C ATOM 1257 OG SER A 86143.061 1.613 -9.227 1.00 0.00 O ATOM 1258 H SER A 86143.057 3.164 -6.555 1.00 0.00 H ATOM 1259 HA SER A 86141.017 1.314 -7.563 1.00 0.00 H ATOM 1260 1HB SER A 86144.035 1.078 -7.518 1.00 0.00 H ATOM 1261 2HB SER A 86142.936 -0.133 -8.178 1.00 0.00 H ATOM 1262 HG SER A 86142.156 1.684 -9.542 1.00 0.00 H ATOM 1263 N CYS A 87141.410 1.178 -4.715 1.00 0.00 N ATOM 1264 CA CYS A 87141.328 0.494 -3.430 1.00 0.00 C ATOM 1265 C CYS A 87139.877 0.215 -3.053 1.00 0.00 C ATOM 1266 O CYS A 87138.984 1.005 -3.360 1.00 0.00 O ATOM 1267 CB CYS A 87141.999 1.331 -2.340 1.00 0.00 C ATOM 1268 SG CYS A 87143.804 1.366 -2.440 1.00 0.00 S ATOM 1269 H CYS A 87141.062 2.090 -4.794 1.00 0.00 H ATOM 1270 HA CYS A 87141.851 -0.446 -3.521 1.00 0.00 H ATOM 1271 1HB CYS A 87141.648 2.350 -2.411 1.00 0.00 H ATOM 1272 2HB CYS A 87141.730 0.931 -1.372 1.00 0.00 H ATOM 1273 HG CYS A 87144.150 1.419 -1.547 1.00 0.00 H ATOM 1274 N ARG A 88139.650 -0.912 -2.386 1.00 0.00 N ATOM 1275 CA ARG A 88138.306 -1.294 -1.967 1.00 0.00 C ATOM 1276 C ARG A 88138.213 -1.371 -0.443 1.00 0.00 C ATOM 1277 O ARGA 88139.151 -1.815 0.220 1.00 0.00 O ATOM 1278 CB ARG A 88137.922 -2.641 -2.582 1.00 0.00 C ATOM 1279 CG ARG A 88137.196 -2.517 -3.912 1.00 0.00 C ATOM 1280 CD ARG A 88135.691 -2.650 -3.741 1.00 0.00 C ATOM 1281 NE ARG A 88135.014 -2.887 -5.014 1.00 0.00 N ATOM 1282 CZ ARG A 88135.048 -4.047 -5.667 1.00 0.00 C ATOM 1283 NH1 ARG A 88135.722 -5.076 -5.171 1.00 0.00 N ATOM 1284 NH2 ARG A 88134.404 -4.178 -6.818 1.00 0.00 N ATOM 1285 H ARG A 88140.403 -1.499 -2.170 1.00 0.00 H ATOM 1286 HA ARG A 88137.622 -0.538 -2.321 1.00 0.00 H ATOM 1287 1HB ARG A 88138.819 -3.221 -2.738 1.00 0.00 H ATOM 1288 2HB ARG A 88137.278 -3.168 -1.893 1.00 0.00 H ATOM 1289 1HG ARG A 88137.415 -1.551 -4.342 1.00 0.00 H ATOM 1290 2HG ARG A 88137.545 -3.296 -4.575 1.00 0.00 H ATOM 1291 1HD ARG A 88135.489 -3.478 -3.078 1.00 0.00 H ATOM 1292 2HD ARG A 88135.310 -1.739 -3.305 1.00 0.00 H ATOM 1293 HE ARG A 88134.509 -2.143 -5.402 1.00 0.00 H ATOM 1294 1HH1 ARG A 88136.210 -4.985 -4.303 1.00 0.00 H ATOM 1295 2HH1 ARG A 88135.743 -5.945 -5.665 1.00 0.00 H ATOM 1296 1HH2 ARG A 88133.894 -3.405 -7.196 1.00 0.00 H ATOM 1297 2HH2 ARG A 88134.428 -5.048 -7.309 1.00 0.00 H ATOM 1298 N PRO A 89137.078 -0.939 0.135 1.00 0.00 N ATOM 1299 CA PRO A 89136.874 -0.966 1.588 1.00 0.00 C ATOM 1300 C PRO A 89137.102 -2.352 2.179 1.00 0.00 C ATOM 1301 O PRO A 89136.511 -3.334 1.728 1.00 0.00 O ATOM 1302 CB PRO A 89135.410 -0.549 1.755 1.00 0.00 C ATOM 1303 CG PRO A 89135.090 0.225 0.523 1.00 0.00 C

ATOM 1304 CD PRO A 89135.907 -0.394 -0.577 1.00 0.00 C ATOM 1305 HA PRO A 89137.513 -0.254 2.089 1.00 0.00 H ATOM 1306 1HB PRO A 89134.791 -1.430 1.841 1.00 0.00 H ATOM 1307 2HB PRO A 89135.305 0.060 2.641 1.00 0.00 H ATOM 1308 1HG PRO A 89134.037 0.140 0.301 1.00 0.00 H ATOM 1309 2HG PRO A 89135.366 1.260 0.658 1.00 0.00 H ATOM 1310 1HD PRO A 89135.351 -1.180 -1.064 1.00 0.00 H ATOM 1311 2HD PRO A 89136.206 0.358 -1.292 1.00 0.00 H ATOM 1312 N ASPA 90137.960 -2.426 3.190 1.00 0.00 N ATOM 1313 CA ASPA 90138.264 -3.694 3.844 1.00 0.00 C ATOM 1314 C ASPA 90137.542 -3.802 5.183 1.00 0.00 C ATOM 1315 O ASPA 90137.962 -3.209 6.176 1.00 0.00 O ATOM 1316 CB ASPA 90139.773 -3.835 4.052 1.00 0.00 C ATOM 1317 CG ASPA 90140.201 -5.279 4.220 1.00 0.00 C ATOM 1318 OD1 ASP A 90140.849 -5.592 5.241 1.00 0.00 O ATOM 1319 OD2 ASP A 90139.886 -6.098 3.331 1.00 0.00 O ATOM 1320 H ASPA 90138.399 -1.609 3.505 1.00 0.00 H ATOM 1321 HA ASP A 90137.923 -4.488 3.199 1.00 0.00 H ATOM 1322 1HB ASP A 90140.288 -3.423 3.197 1.00 0.00 H ATOM 1323 2HB ASP A 90140.061 -3.287 4.937 1.00 0.00 H ATOM 1324 N SER A 91136.454 -4.564 5.202 1.00 0.00 N ATOM 1325 CA SER A 91135.673 -4.751 6.420 1.00 0.00 C ATOM 1326 C SER A 91136.034 -6.066 7.101 1.00 0.00 C ATOM 1327 O SER A 91135.196 -6.689 7.753 1.00 0.00 O ATOM 1328 CB SER A 91134.177 -4.723 6.101 1.00 0.00 C ATOM 1329 OG SER A 91133.431 -4.222 7.197 1.00 0.00 O ATOM 1330 H SER A 91136.168 -5.012 4.378 1.00 0.00 H ATOM 1331 HA SER A 91135.904 -3.937 7.090 1.00 0.00 H ATOM 1332 1HB SER A 91134.005 -4.088 5.245 1.00 0.00 H ATOM 1333 2HB SER A 91133.841 -5.725 5.881 1.00 0.00 H ATOM 1334 HG SER A 91133.583 -3.278 7.284 1.00 0.00 H

ATOM 1335 N ARG A 92137.285 -6.486 6.944 1.00 0.00 N ATOM 1336 CA ARG A 92137.756 -7.728 7.544 1.00 0.00 C ATOM 1337 C ARG A 92137.792 -7.619 9.064 1.00 0.00 C ATOM 1338 O ARG A 92137.609 -8.610 9.772 1.00 0.00 O ATOM 1339 CB ARG A 92139.148 -8.079 7.013 1.00 0.00 C ATOM 1340 CG ARG A 92139.143 -8.589 5.580 1.00 0.00 C ATOM 1341 CD ARG A 92139.469 -10.073 5.512 1.00 0.00 C ATOM 1342 NE ARG A 92138.336 -10.902 5.917 1.00 0.00 N ATOM 1343 CZ ARG A 92138.226 -12.197 5.630 1.00 0.00 C ATOM 1344 NH1 ARG A 92139.176 -12.813 4.938 1.00 0.00 N ATOM 1345 NH2 ARG A 92137.162 -12.877 6.034 1.00 0.00 N ATOM 1346 H ARG A 92137.907 -5.946 6.412 1.00 0.00 H ATOM 1347 HA ARG A 92137.067 -8.511 7.267 1.00 0.00 H ATOM 1348 1HB ARG A 92139.770 -7.197 7.057 1.00 0.00 H ATOM 1349 2HB ARG A 92139.579 -8.843 7.644 1.00 0.00 H ATOM 1350 1HG ARG A 92138.163 -8.427 5.155 1.00 0.00 H ATOM 1351 2HG ARG A 92139.879 -8.040 5.012 1.00 0.00 H ATOM 1352 1HD ARG A 92139.739 -10.322 4.497 1.00 0.00 H ATOM 1353 2HD ARG A 92140.303 -10.275 6.167 1.00 0.00 H ATOM 1354 HE ARG A 92137.620 -10.471 6.430 1.00 0.00 H ATOM 1355 1HH1 ARG A 92139.980 -12.307 4.629 1.00 0.00 H ATOM 1356 2HH1 ARG A 92139.088 -13.787 4.725 1.00 0.00 H ATOM 1357 1HH2 ARG A 92136.443 -12.418 6.556 1.00 0.00 H ATOM 1358 2HH2 ARG A 92137.079 -13.850 5.819 1.00 0.00 H ATOM 1359 N PHE A 93138.031 -6.410 9.561 1.00 0.00 N ATOM 1360 CA PHE A 93138.092 -6.172 10.999 1.00 0.00 C ATOM 1361 C PHE A 93136.976 -5.233 11.447 1.00 0.00 C ATOM 1362 O PHE A 93137.114 -4.519 12.440 1.00 0.00 O ATOM 1363 CB PHE A 93139.451 -5.583 11.381 1.00 0.00 C ATOM 1364 CG PHE A 93140.586 -6.559 11.253 1.00 0.00 C ATOM 1365 CD1 PHE A 93140.898 -7.122 10.026 1.00 0.00 C

ATOM 1366 CD2 PHE A 93141.340 -6.914 12.361 1.00 0.00 C ATOM 1367 CE1 PHE A 93141.942 -8.020 9.905 1.00 0.00 C ATOM 1368 CE2 PHE A 93142.385 -7.811 12.246 1.00 0.00 C ATOM 1369 CZ PHE A 93142.686 -8.365 11.017 1.00 0.00 C ATOM 1370 H PHE A 93138.170 -5.659 8.947 1.00 0.00 H ATOM 1371 HA PHE A 93137.968 -7.122 11.497 1.00 0.00 H ATOM 1372 1HB PHE A 93139.664 -4.741 10.740 1.00 0.00 H ATOM 1373 2HB PHE A 93139.413 -5.248 12.407 1.00 0.00 H ATOM 1374 HD1 PHE A 93140.317 -6.853 9.156 1.00 0.00 H ATOM 1375 HD2 PHE A 93141.105 -6.482 13.322 1.00 0.00 H ATOM 1376 HE1 PHE A 93142.175 -8.451 8.944 1.00 0.00 H ATOM 1377 HE2 PHE A 93142.965 -8.079 13.117 1.00 0.00 H ATOM 1378 HZ PHE A 93143.502 -9.066 10.925 1.00 0.00 H ATOM 1379 N ALA A 94135.869 -5.238 10.710 1.00 0.00 N ATOM 1380 CA ALA A 94134.732 -4.386 11.038 1.00 0.00 C ATOM 1381 C ALA A 94133.628 -5.181 11.726 1.00 0.00 C ATOM 1382 O ALAA 94133.159 -6.193 11.204 1.00 0.00 O ATOM 1383 CB ALAA 94134.197 -3.716 9.780 1.00 0.00 C ATOM 1384 H ALAA 94135.814 -5.829 9.930 1.00 0.00 H ATOM 1385 HA ALA A 94135.077 -3.614 11.709 1.00 0.00 H ATOM 1386 1HB ALA A 94133.322 -4.246 9.434 1.00 0.00 H ATOM 1387 2HB ALA A 94134.956 -3.732 9.013 1.00 0.00 H ATOM 1388 3HB ALA A 94133.932 -2.693 10.004 1.00 0.00 H ATOM 1389 N SER A 95133.216 -4.717 12.902 1.00 0.00 N ATOM 1390 CA SER A 95132.167 -5.384 13.663 1.00 0.00 C ATOM 1391 C SER A 95130.804 -4.767 13.363 1.00 0.00 C ATOM 1392 O SER A 95130.659 -3.546 13.331 1.00 0.00 O ATOM 1393 CB SER A 95132.460 -5.298 15.162 1.00 0.00 C ATOM 1394 OG SER A 95133.403 -6.280 15.554 1.00 0.00 O ATOM 1395 H SER A 95133.629 -3.905 13.266 1.00 0.00 H ATOM 1396 HA SER A 95132.152 -6.422 13.366 1.00 0.00 H

ATOM 1397 1HB SER A 95132.860 -4.322 15.392 1.00 0.00 H ATOM 1398 2HB SER A 95131.546 -5.452 15.714 1.00 0.00 H ATOM 1399 HG SER A 95132.941 -7.050 15.894 1.00 0.00 H ATOM 1400 N LEU A 96129.809 -5.620 13.143 1.00 0.00 N ATOM 1401 CA LEU A 96128.459 -5.157 12.847 1.00 0.00 C ATOM 1402 C LEUA 96127.448 -6.288 13.000 1.00 0.00 C ATOM 1403 O LEUA 96127.601 -7.357 12.405 1.00 0.00 O ATOM 1404 CB LEU A 96128.394 -4.589 11.428 1.00 0.00 C ATOM 1405 CG LEU A 96127.019 -4.076 10.997 1.00 0.00 C ATOM 1406 CD1 LEU A 96126.635 -2.843 11.801 1.00 0.00 C ATOM 1407 CD2 LEU A 96127.009 -3.769 9.507 1.00 0.00 C ATOM 1408 H LEU A 96129.987 -6.583 13.183 1.00 0.00 H ATOM 1409 HA LEU A 96128.215 -4.375 13.549 1.00 0.00 H ATOM 1410 1HB LEU A 96129.099 -3.773 11.358 1.00 0.00 H ATOM 1411 2HB LEU A 96128.696 -5.363 10.738 1.00 0.00 H ATOM 1412 HG LEU A 96126.281 -4.841 11.187 1.00 0.00 H ATOM 1413 1HD1 LEU A 96126.375 -3.136 12.807 1.00 0.00 H ATOM 1414 2HD1 LEU A 96125.788 -2.360 11.336 1.00 0.00 H ATOM 1415 3HD1 LEU A 96127.468 -2.157 11.829 1.00 0.00 H ATOM 1416 1HD2 LEU A 96127.887 -3.195 9.252 1.00 0.00 H ATOM 1417 2HD2 LEU A 96126.124 -3.200 9.263 1.00 0.00 H ATOM 1418 3HD2 LEU A 96127.008 -4.693 8.949 1.00 0.00 H ATOM 1419 N GLN A 97126.414 -6.047 13.800 1.00 0.00 N ATOM 1420 CA GLN A 97125.375 -7.044 14.031 1.00 0.00 C ATOM 1421 C GLN A 97124.046 -6.595 13.432 1.00 0.00 C ATOM 1422 O GLN A 97123.770 -5.398 13.339 1.00 0.00 O ATOM 1423 CB GLN A 97125.212 -7.303 15.529 1.00 0.00 C ATOM 1424 CG GLN A 97126.300 -8.185 16.117 1.00 0.00 C ATOM 1425 CD GLN A 97126.152 -9.640 15.720 1.00 0.00 C ATOM 1426 OE1 GLN A 97125.213 -10.317 16.141 1.00 0.00 O ATOM 1427 NE2 GLN A 97127.077 -10.129 14.903 1.00 0.00 N ATOM 1428 H GLN A 97126.347 -5.176 14.244 1.00 0.00 H ATOM 1429 HA GLN A 97125.682 -7.961 13.548 1.00 0.00 H ATOM 1430 1HB GLN A 97125.225 -6.356 16.050 1.00 0.00 H ATOM 1431 2HB GLN A 97124.259 -7.784 15.699 1.00 0.00 H ATOM 1432 1HG GLN A 97127.260 -7.830 15.771 1.00 0.00 H ATOM 1433 2HG GLN A 97126.260 -8.115 17.196 1.00 0.00 H ATOM 1434 1HE2 GLN A 97127.796 -9.531 14.608 1.00 0.00 H ATOM 1435 2HE2 GLN A 97127.005 -11.066 14.630 1.00 0.00 H ATOM 1436 N PRO A 98123.198 -7.552 13.015 1.00 0.00 N ATOM 1437 CA PRO A 98121.892 -7.248 12.423 1.00 0.00 C ATOM 1438 C PRO A 98121.064 -6.310 13.296 1.00 0.00 C ATOM 1439 O PRO A 98121.520 -5.859 14.346 1.00 0.00 O ATOM 1440 CB PRO A 98121.218 -8.617 12.320 1.00 0.00 C ATOM 1441 CG PRO A 98122.345 -9.589 12.252 1.00 0.00 C ATOM 1442 CD PRO A 98123.448 -9.004 13.089 1.00 0.00 C ATOM 1443 HA PRO A 98121.996 -6.819 11.436 1.00 0.00 H ATOM 1444 1HB PRO A 98120.603 -8.785 13.193 1.00 0.00 H ATOM 1445 2HB PRO A 98120.610 -8.657 11.430 1.00 0.00 H ATOM 1446 1HG PRO A 98122.033 -10.541 12.655 1.00 0.00 H ATOM 1447 2HG PRO A 98122.671 -9.702 11.228 1.00 0.00 H ATOM 1448 1HD PRO A 98123.376 -9.356 14.108 1.00 0.00 H ATOM 1449 2HD PRO A 98124.412 -9.251 12.670 1.00 0.00 H ATOM 1450 N SER A 99119.844 -6.023 12.855 1.00 0.00 N ATOM 1451 CA SER A 99118.951 -5.140 13.597 1.00 0.00 C ATOM 1452 C SER A 99117.810 -5.928 14.232 1.00 0.00 C ATOM 1453 O SER A 99117.697 -5.997 15.456 1.00 0.00 O ATOM 1454 CB SER A 99118.386 -4.058 12.675 1.00 0.00 C ATOM 1455 OG SER A 99118.327 -4.512 11.333 1.00 0.00 O ATOM 1456 H SER A 99119.535 -6.414 12.011 1.00 0.00 H ATOM 1457 HA SER A 99119.527 -4.669 14.379 1.00 0.00 H ATOM 1458 1HB SER A 99117.390 -3.797 12.997 1.00 0.00 H

ATOM 1459 2HB SER A 99119.020 -3.184 12.717 1.00 0.00 H ATOM 1460 HG SER A 99118.412 -3.764 10.737 1.00 0.00 H ATOM 1461 N GLY A 100116.966 -6.519 13.393 1.00 0.00 N ATOM 1462 CA GLY A 100115.846 -7.293 13.892 1.00 0.00 C ATOM 1463 C GLY A 100114.524 -6.565 13.742 1.00 0.00 C ATOM 1464 O GLY A 100114.144 -5.782 14.613 1.00 0.00 O ATOM 1465 H GLY A 100117.107 -6.428 12.427 1.00 0.00 H ATOM 1466 1HA GLY A 100115.796 -8.225 13.347 1.00 0.00 H ATOM 1467 2HA GLY A 100116.009 -7.509 14.937 1.00 0.00 H ATOM 1468 N° PRO A 101113.793 -6.802 12.638 1.00 0.00 N ATOM 1469 CA PRO A 101112.500 -6.153 12.392 1.00 0.00 C ATOM 1470 C PRO A 101111.553 -6.277 13.581 1.00 0.00 C ATOM 1471 O PRO A 101111.276 -7.378 14.055 1.00 0.00 O ATOM 1472 CB PRO A 101111.946 -6.912 11.186 1.00 0.00 C ATOM 1473 CG PRO A 101113.151 -7.427 10.478 1.00 0.00 C ATOM 1474 CD PRO A 101114.167 -7.720 11.546 1.00 0.00 C ATOM 1475 HA PRO A 101112.624 -5.110 12.139 1.00 0.00 H ATOM 1476 1HB PRO A 101111.311 -7.718 11.525 1.00 0.00 H ATOM 1477 2HB PRO A 101111.380 -6.238 10.561 1.00 0.00 H ATOM 1478 1HG PRO A 101112.901 -8.329 9.939 1.00 0.00 H ATOM 1479 2HG PRO A 101113.526 -6.676 9.799 1.00 0.00 H ATOM 1480 1HD PRO A 101114.093 -8.749 11.865 1.00 0.00 H ATOM 1481 2HD PRO A 101115.164 -7.505 11.188 1.00 0.00 H ATOM 1482 N SER A 102111.061 -5.138 14.060 1.00 0.00 N ATOM 1483 CA SER A 102110.144 -5.120 15.194 1.00 0.00 C ATOM 1484 C SER A 102110.802 -5.719 16.434 1.00 0.00 C ATOM 1485 O SER A 102110.493 -6.842 16.831 1.00 0.00 O ATOM 1486 CB SER A 102108.866 -5.890 14.857 1.00 0.00 C ATOM 1487 OG SER A 102107.873 -5.024 14.333 1.00 0.00 O ATOM 1488 H SER A 102111.319 -4.292 13.640 1.00 0.00 H ATOM 1489 HA SER A 102109.891 -4.091 15.398 1.00 0.00 H

ATOM 1490 1HB SER A 102109.088 -6.647 14.120 1.00 0.00 H ATOM 1491 2HB SER A 102108.483 -6.358 15.752 1.00 0.00 H ATOM 1492 HG SER A 102108.270 -4.434 13.690 1.00 0.00 H ATOM 1493 N SER A 103111.709 -4.961 17.041 1.00 0.00 N ATOM 1494 CA SER A 103112.410 -5.416 18.235 1.00 0.00 C ATOM 1495 C SER A 103111.554 -5.208 19.481 1.00 0.00 C ATOM 1496 O SER A 103110.663 -4.359 19.498 1.00 0.00 O ATOM 1497 CB SER A 103113.740 -4.676 18.385 1.00 0.00 C ATOM 1498 OG SER A 103114.772 -5.329 17.666 1.00 0.00 O ATOM 1499 H SER A 103111.912 -4.075 16.676 1.00 0.00 H ATOM 1500 HA SER A 103112.607 -6.472 18.121 1.00 0.00 H ATOM 1501 1HB SER A 103113.634 -3.670 18.006 1.00 0.00 H ATOM 1502 2HB SER A 103114.013 -4.638 19.430 1.00 0.00 H ATOM 1503 HG SER A 103114.839 -6.240 17.960 1.00 0.00 H ATOM 1504 N GLY A 104111.832 -5.986 20.520 1.00 0.00 N ATOM 1505 CA GLY A 104111.079 -5.871 21.756 1.00 0.00 C ATOM 1506 C GLY A 104111.969 -5.896 22.983 1.00 0.00 C ATOM 1507 O GLY A 104111.575 -6.523 23.989 1.00 0.00 O ATOM 1508 OXT GLY A 104113.061 -5.291 22.937 1.00 0.00 O ATOM 1509 H GLY A 104112.555 -6.645 20.449 1.00 0.00 H ATOM 1510 1HA GLY A 104110.529 -4.941 21.743 1.00 0.00 H ATOM 1511 2HA GLY A 104110.379 -6.691 21.815 1.00 0.00 H TER 1512 GLY A 104 **ENDMDL**

Three-Dimensional Structure Coordinate Table 10

ATOM 1 N GLY A 1132.485 -2.135 -14.848 1.00 0.00 N ATOM 2 CA GLY A 1133.474 -2.831 -13.979 1.00 0.00 C ATOM 3 C GLY A 1133.260 -2.538 -12.507 1.00 0.00 C ATOM 4 O GLY A 1133.286 -3.446 -11.676 1.00 0.00 O ATOM 5 1H GLY A 1132.906 -1.268 -15.244 1.00 0.00 H ATOM 6 2H GLY A 1131.643 -1.877 -14.296 1.00 0.00 H ATOM 7 3H GLY A 1132.197 -2.756 -15.631 1.00 0.00 H ATOM 8 1HA GLY A 1133.389 -3.896 -14.138 1.00 0.00 H ATOM 9 2HA GLY A 1134.468 -2.515 -14.257 1.00 0.00 H ATOM10 N SER A 2133.048 -1.266 -12.184 1.00 0.00 N ATOM11 CA SER A 2132.829 -0.855 -10.803 1.00 0.00 C ATOM12 C SER A 2131.367 -0.493 -10.568 1.00 0.00 C ATOM13 O SER A 2130.763 0.238 -11.354 1.00 0.00 O ATOM14 CB SER A 2133.723 0.338 -10.456 1.00 0.00 C ATOM15 OG SER A 2133.256 1.523 -11.074 1.00 0.00 O ATOM16 H SER A 2133.039 -0.588 -12.892 1.00 0.00 H ATOM17 HA SER A 2133.089 -1.686 -10.164 1.00 0.00 H ATOM18 1HB SER A 2133.727 0.483 -9.386 1.00 0.00 H ATOM19 2HB SER A 2134.729 0.141 -10.795 1.00 0.00 H ATOM20 HG SER A 2133.668 2.285 -10.661 1.00 0.00 H ATOM21 N SER A 3130.801 -1.010 -9.482 1.00 0.00 N ATOM22 CA SER A 3129.408 -0.742 -9.143 1.00 0.00 C ATOM23 C SER A 3129.287 0.525 -8.303 1.00 0.00 C ATOM24 O SER A 3129.369 0.478 -7.076 1.00 0.00 O ATOM25 CB SER A 3128.807 -1.928 -8.388 1.00 0.00 C ATOM26 OG SER A 3127.458 -2.142 -8.764 1.00 0.00 O ATOM27 H SER A 3131.334 -1.586 -8.893 1.00 0.00 H ATOM28 HA SER A 3128.865 -0.602 -10.066 1.00 0.00 H ATOM29 1HB SER A 3129.375 -2.820 -8.612 1.00 0.00 H ATOM30 2HB SER A 3128.847 -1.734 -7.326 1.00 0.00 H ATOM31 HG SER A 3126.975 -1.313 -8.709 1.00 0.00 H ATOM32 N GLY A 4129.091 1.657 -8.972 1.00 0.00 N ATOM33 CA GLY A 4128.962 2.919 -8.271 1.00 0.00 C ATOM34 C GLY A 4128.420 4.023 -9.158 1.00 0.00 C ATOM35 O GLY A 4128.458 3.918 -10.383 1.00 0.00 O ATOM36 H GLY A 4129.035 1.633 -9.950 1.00 0.00 H

ATOM37 1HA GLY A 4128.293 2.787 -7.432 1.00 0.00 H ATOM38 2HA GLY A 4129.932 3.214 -7.901 1.00 0.00 H ATOM39 N SER A 5127.915 5.084 -8.537 1.00 0.00 N ATOM40 CA SER A 5127.362 6.212 -9.279 1.00 0.00 C ATOM41 C SER A 5127.409 7.487 -8.444 1.00 0.00 C ATOM42 O SER A 5127.856 8.534 -8.914 1.00 0.00 O ATOM43 CB SER A 5125.922 5.916 -9.699 1.00 0.00 C ATOM44 OG SER A 5125.076 5.793 -8.569 1.00 0.00 O ATOM45 H SER A 5127.913 5.110 -7.558 1.00 0.00 H ATOM46 HA SER A 5127.964 6.353 -10.164 1.00 0.00 H ATOM47 1HB SER A 5125.558 6.722 -10.319 1.00 0.00 H ATOM48 2HB SER A 5125.895 4.993 -10.258 1.00 0.00 H ATOM49 HG SER A 5124.212 6.159 -8.774 1.00 0.00 H ATOM50 N SER A 6126.945 7.394 -7.202 1.00 0.00 N ATOM51 CA SER A 6126.933 8.540 -6.301 1.00 0.00 C ATOM52 C SER A 6128.282 8.699 -5.606 1.00 0.00 C ATOM53 O SER A 6129.041 7.739 -5.475 1.00 0.00 O ATOM54 CB SER A 6125.824 8.385 -5.259 1.00 0.00 C ATOM55 OG SER A 6125.843 7.091 -4.683 1.00 0.00 O ATOM56 H SER A 6126.601 6.532 -6.884 1.00 0.00 H ATOM57 HA SER A 6126.740 9.423 -6.892 1.00 0.00 H ATOM58 1HB SER A 6125.965 9.115 -4.475 1.00 0.00 H ATOM59 2HB SER A 6124.866 8.543 -5.731 1.00 0.00 H ATOM60 HG SER A 6126.724 6.899 -4.353 1.00 0.00 H ATOM61 N GLYA 7128.574 9.917 -5.163 1.00 0.00 N ATOM62 CA GLY A 7129.830 10.179 -4.487 1.00 0.00 C ATOM63 C GLY A 7129.885 11.568 -3.882 1.00 0.00 C ATOM64 O GLY A 7130.880 12.278 -4.029 1.00 0.00 O ATOM65 H GLY A 7127.930 10.645 -5.297 1.00 0.00 H ATOM66 1HA GLY A 7129.962 9.451 -3.702 1.00 0.00 H ATOM67 2HA GLY A 7130.637 10.078 -5.198 1.00 0.00 H ATOM68 N LEUA 8128.813 11.957 -3.200 1.00 0.00 N ATOM69 CA LEU A 8128.741 13.271 -2.570 1.00 0.00 C ATOM70 C LEUA 8128.749 13.146 -1.050 1.00 0.00 C ATOM71 O LEUA 8128.123 13.940 -0.349 1.00 0.00 O ATOM72 CB LEU A 8127.482 14.011 -3.026 1.00 0.00 C ATOM73 CG LEU A 8127.632 14.802 -4.326 1.00 0.00 C ATOM74 CD1 LEU A 8126.291 14.925 -5.034 1.00 0.00 C ATOM75 CD2 LEU A 8128.217 16.179 -4.047 1.00 0.00 C ATOM76 H LEUA 8128.050 11.347 -3.119 1.00 0.00 H ATOM77 HA LEU A 8129.610 13.834 -2.878 1.00 0.00 H ATOM78 1HB LEU A 8126.692 13.286 -3.158 1.00 0.00 H ATOM79 2HB LEU A 8127.190 14.697 -2.245 1.00 0.00 H ATOM80 HG LEU A 8128.308 14.277 -4.983 1.00 0.00 H ATOM81 1HD1 LEU A 8126.239 15.875 -5.546 1.00 0.00 H ATOM82 2HD1 LEU A 8125.493 14.863 -4.307 1.00 0.00 H ATOM83 3HD1 LEU A 8126.187 14.124 -5.750 1.00 0.00 H ATOM84 1HD2 LEU A 8127.824 16.888 -4.760 1.00 0.00 H ATOM85 2HD2 LEU A 8129.293 16.137 -4.136 1.00 0.00 H ATOM86 3HD2 LEU A 8127.950 16.487 -3.047 1.00 0.00 H ATOM87 N ALAA 9129.465 12.144 -0.548 1.00 0.00 N ATOM88 CA ALA A 9129.555 11.916 0.889 1.00 0.00 C ATOM89 C ALA A 9130.916 11.341 1.267 1.00 0.00 C ATOM90 O ALAA 9131.007 10.386 2.039 1.00 0.00 O ATOM91 CB ALA A 9128.440 10.988 1.346 1.00 0.00 C ATOM92 H ALAA 9129.942 11.546 -1.158 1.00 0.00 H ATOM93 HA ALA A 9129.426 12.866 1.386 1.00 0.00 H ATOM94 1HB ALA A 9128.296 11.095 2.411 1.00 0.00 H ATOM95 2HB ALA A 9128.707 9.966 1.120 1.00 0.00 H ATOM96 3HB ALA A 9127.526 11.242 0.831 1.00 0.00 H ATOM97 N MET A 10131.974 11.929 0.717 1.00 0.00 N ATOM98 CA MET A 10133.332 11.475 0.996 1.00 0.00 C

ATOM99 C MET A 10134.283 12.661 1.158 1.00 0.00 C 100 O META 10135.242 12.808 0.401 1.00 0.00 O ATOM 101 CB META 10133.825 10.557 -0.127 1.00 0.00 C **ATOM** 102 CG META 10133.494 11.064 -1.523 1.00 0.00 C ATOM **ATOM** 103 SD META 10134.899 11.857 -2.329 1.00 0.00 S 104 CE META 10134.803 11.137 -3.965 1.00 0.00 C **ATOM** 105 H META 10131.838 12.686 0.109 1.00 0.00 H **ATOM** 106 HA META 10133.311 10.918 1.920 1.00 0.00 H **ATOM** 107 1HB MET A 10134.897 10.458 -0.048 1.00 0.00 H **ATOM ATOM** 108 2HB MET A 10133.372 9.584 -0.004 1.00 0.00 H 109 1HG MET A 10133.178 10.227 -2.128 1.00 0.00 H **ATOM** 110 2HG MET A 10132.687 11.778 -1.452 1.00 0.00 H ATOM 111 1HE META 10135.673 11.424 -4.536 1.00 0.00 H ATOM 112 2HE MET A 10133.912 11.489 -4.462 1.00 0.00 H **ATOM ATOM** 113 3HE MET A 10134.767 10.060 -3.883 1.00 0.00 H 114 N PRO A 11134.028 13.530 2.154 1.00 0.00 N **ATOM** 115 CA PRO A 11134.869 14.707 2.406 1.00 0.00 C **ATOM** 116 C PRO A 11136.323 14.343 2.706 1.00 0.00 C ATOM 117 O PRO A 11137.243 14.934 2.142 1.00 0.00 O **ATOM** 118 CB PRO A 11134.223 15.370 3.629 1.00 0.00 C **ATOM** 119 CG PRO A 11132.840 14.818 3.694 1.00 0.00 C **ATOM** 120 CD PRO A 11132.907 13.439 3.104 1.00 0.00 C **ATOM** 121 HA PRO A 11134.841 15.391 1.570 1.00 0.00 H **ATOM** 122 1HB PRO A 11134.789 15.125 4.514 1.00 0.00 H **ATOM ATOM** 123 2HB PRO A 11134.212 16.441 3.492 1.00 0.00 H 124 1HG PRO A 11132.515 14.768 4.723 1.00 0.00 H ATOM 125 2HG PRO A 11132.170 15.439 3.119 1.00 0.00 H **ATOM** 126 1HD PRO A 11133.108 12.708 3.873 1.00 0.00 H **ATOM** 127 2HD PRO A 11131.985 13.205 2.592 1.00 0.00 H ATOM 128 N PRO A 12136.556 13.370 3.608 1.00 0.00 N **ATOM** 129 CA PRO A 12137.907 12.949 3.978 1.00 0.00 C ATOM

130 C PROA 12138.499 11.939 3.000 1.00 0.00 C ATOM 131 O PROA 12139.664 12.044 2.616 1.00 0.00 O **ATOM** 132 CB PRO A 12137.694 12.306 5.345 1.00 0.00 C ATOM 133 CG PRO A 12136.322 11.725 5.275 1.00 0.00 C **ATOM** 134 CD PRO A 12135.527 12.609 4.344 1.00 0.00 C **ATOM** 135 HA PRO A 12138.574 13.792 4.073 1.00 0.00 H **ATOM ATOM** 136 1HB PRO A 12138.441 11.543 5.507 1.00 0.00 H 137 2HB PRO A 12137.765 13.059 6.116 1.00 0.00 H **ATOM ATOM** 138 1HG PRO A 12136.371 10.720 4.885 1.00 0.00 H 139 2HG PRO A 12135.876 11.724 6.259 1.00 0.00 H **ATOM** 140 1HD PRO A 12134.939 12.007 3.668 1.00 0.00 H **ATOM ATOM** 141 2HD PRO A 12134.889 13.271 4.910 1.00 0.00 H 142 N GLY A 13137.695 10.958 2.605 1.00 0.00 N **ATOM** 143 CA GLY A 13138.165 9.942 1.680 1.00 0.00 C ATOM 144 C GLYA 13137.387 9.927 0.380 1.00 0.00 C **ATOM** 145 O GLYA 13137.055 10.980 -0.165 1.00 0.00 O **ATOM** 146 H GLY A 13136.776 10.921 2.947 1.00 0.00 H **ATOM** 147 1HA GLY A 13139.206 10.126 1.460 1.00 0.00 H ATOM 148 2HA GLY A 13138.075 8.975 2.152 1.00 0.00 H **ATOM** 149 N ASNA 14137.097 8.729 -0.117 1.00 0.00 N **ATOM** 150 CA ASN A 14136.354 8.576 -1.364 1.00 0.00 C **ATOM** 151 C ASNA 14135.392 7.395 -1.282 1.00 0.00 C **ATOM** 152 O ASNA 14135.721 6.353 -0.716 1.00 0.00 O ATOM 153 CB ASN A 14137.318 8.384 -2.536 1.00 0.00 C **ATOM** 154 CG ASN A 14138.440 9.403 -2.536 1.00 0.00 C **ATOM** 155 OD1 ASN A 14138.425 10.362 -3.307 1.00 0.00 O **ATOM** 156 ND2 ASN A 14139.424 9.201 -1.666 1.00 0.00 N **ATOM** 157 H ASN A 14137.390 7.928 0.364 1.00 0.00 H **ATOM** 158 HA ASN A 14135.785 9.479 -1.523 1.00 0.00 H **ATOM** 159 1HB ASN A 14137.753 7.397 -2.478 1.00 0.00 H **ATOM** 160 2HB ASN A 14136.771 8.478 -3.462 1.00 0.00 H **ATOM**

161 1HD2 ASN A 14139.370 8.415 -1.082 1.00 0.00 H **ATOM ATOM** 162 2HD2 ASN A 14140.162 9.844 -1.644 1.00 0.00 H 163 N SER A 15134.203 7.567 -1.851 1.00 0.00 N **ATOM** 164 CA SER A 15133.189 6.517 -1.845 1.00 0.00 C **ATOM** 165 C SER A 15132.729 6.212 -0.422 1.00 0.00 C **ATOM** 166 O SER A 15131.666 6.664 0.007 1.00 0.00 O **ATOM** 167 CB SER A 15133.733 5.247 -2.504 1.00 0.00 C **ATOM** 168 OG SER A 15133.356 5.179 -3.869 1.00 0.00 O **ATOM** 169 H SER A 15134.001 8.422 -2.287 1.00 0.00 H **ATOM** 170 HA SER A 15132.344 6.872 -2.414 1.00 0.00 H **ATOM** 171 1HB SER A 15134.811 5.244 -2.442 1.00 0.00 H **ATOM** 172 2HB SER A 15133.341 4.381 -1.991 1.00 0.00 H **ATOM ATOM** 173 HG SER A 15132.415 5.352 -3.950 1.00 0.00 H 174 N HIS A 16133.533 5.445 0.306 1.00 0.00 N ATOM 175 CA HIS A 16133.208 5.082 1.680 1.00 0.00 C **ATOM** 176 C HIS A 16134.066 5.865 2.668 1.00 0.00 C **ATOM** 177 O HIS A 16133.573 6.351 3.686 1.00 0.00 O **ATOM ATOM** 178 CB HIS A 16133.405 3.580 1.894 1.00 0.00 C 179 CG HIS A 16132.249 2.752 1.423 1.00 0.00 C **ATOM** 180 ND1 HIS A 16131.753 1.680 2.135 1.00 0.00 N **ATOM** 181 CD2 HIS A 16131.490 2.843 0.305 1.00 0.00 C **ATOM** 182 CE1 HIS A 16130.739 1.148 1.475 1.00 0.00 C **ATOM** 183 NE2 HIS A 16130.560 1.835 0.362 1.00 0.00 N **ATOM ATOM** 184 H HIS A 16134.367 5.115 -0.090 1.00 0.00 H 185 HA HIS A 16132.170 5.328 1.851 1.00 0.00 H **ATOM** 186 1HB HIS A 16134.284 3.260 1.355 1.00 0.00 H **ATOM** 187 2HB HIS A 16133.545 3.389 2.948 1.00 0.00 H **ATOM** 188 HD1 HIS A 16132.093 1.357 2.995 1.00 0.00 H **ATOM** 189 HD2 HIS A 16131.598 3.573 -0.485 1.00 0.00 H **ATOM** 190 HE1 HIS A 16130.157 0.295 1.792 1.00 0.00 H **ATOM** 191 HE2 HIS A 16129.823 1.704 -0.270 1.00 0.00 H ATOM

192 N GLYA 17135.354 5.982 2.360 1.00 0.00 N ATOM 193 CA GLY A 17136.261 6.707 3.230 1.00 0.00 C **ATOM** 194 C GLYA 17137.602 6.015 3.375 1.00 0.00 C ATOM 195 O GLYA 17138.004 5.653 4.481 1.00 0.00 O **ATOM** 196 H GLY A 17135.690 5.574 1.536 1.00 0.00 H **ATOM** 197 1HA GLY A 17136.421 7.695 2.823 1.00 0.00 H **ATOM** ATOM 198 2HA GLY A 17135.809 6.802 4.206 1.00 0.00 H 199 N LEUA 18138.294 5.830 2.256 1.00 0.00 N **ATOM** 200 CA LEU A 18139.598 5.176 2.264 1.00 0.00 C **ATOM** 201 C LEUA 18140.706 6.174 2.579 1.00 0.00 C **ATOM** 202 O LEUA 18141.119 6.952 1.718 1.00 0.00 O ATOM 203 CB LEU A 18139.865 4.509 0.913 1.00 0.00 C **ATOM** 204 CG LEU A 18138.793 3.519 0.456 1.00 0.00 C **ATOM** 205 CD1 LEU A 18138.995 3.149 -1.004 1.00 0.00 C **ATOM** 206 CD2 LEU A 18138.812 2.274 1.330 1.00 0.00 C **ATOM** 207 H LEUA 18137.921 6.141 1.406 1.00 0.00 H **ATOM** 208 HA LEU A 18139.583 4.418 3.032 1.00 0.00 H **ATOM** 209 1HB LEU A 18139.953 5.284 0.165 1.00 0.00 H **ATOM** 210 2HB LEU A 18140.806 3.983 0.975 1.00 0.00 H **ATOM** 211 HG LEUA 18137.821 3.981 0.552 1.00 0.00 H ATOM 212 1HD1 LEU A 18139.946 2.651 -1.122 1.00 0.00 H ATOM 213 2HD1 LEU A 18138.982 4.045 -1.608 1.00 0.00 H **ATOM** 214 3HD1 LEU A 18138.202 2.489 -1.322 1.00 0.00 H ATOM 215 1HD2 LEU A 18139.397 1.505 0.849 1.00 0.00 H ATOM 216 2HD2 LEU A 18137.802 1.920 1.475 1.00 0.00 H **ATOM** 217 3HD2 LEU A 18139.250 2.513 2.288 1.00 0.00 H ATOM 218 N GLUA 19141.185 6.148 3.819 1.00 0.00 N ATOM 219 CA GLU A 19142.246 7.051 4.248 1.00 0.00 C ATOM 220 C GLUA 19143.202 6.348 5.207 1.00 0.00 C ATOM 221 O GLUA 19143.061 5.156 5.479 1.00 0.00 O **ATOM** 222 CB GLU A 19141.650 8.289 4.919 1.00 0.00 C ATOM

223 CG GLU A 19140.820 7.972 6.152 1.00 0.00 C **ATOM** 224 CD GLUA 19141.049 8.961 7.279 1.00 0.00 C **ATOM** 225 OE1 GLU A 19142.219 9.330 7.517 1.00 0.00 O **ATOM ATOM** 226 OE2 GLU A 19140.058 9.368 7.922 1.00 0.00 O 227 H GLUA 19140.816 5.504 4.460 1.00 0.00 H ATOM **ATOM** 228 HA GLU A 19142.796 7.357 3.371 1.00 0.00 H 229 1HB GLU A 19142.455 8.948 5.212 1.00 0.00 H **ATOM ATOM** 230 2HB GLUA 19141.018 8.800 4.209 1.00 0.00 H **ATOM** 231 1HG GLUA 19139.776 7.993 5.883 1.00 0.00 H 232 2HG GLUA 19141.081 6.984 6.502 1.00 0.00 H **ATOM** 233 N VALA 20144.175 7.096 5.717 1.00 0.00 N **ATOM** 234 CA VALA 20145.156 6.545 6.647 1.00 0.00 C **ATOM ATOM** 235 C VALA 20144.476 5.973 7.886 1.00 0.00 C **ATOM** 236 O VALA 20143.563 6.582 8.443 1.00 0.00 O 237 CB VALA 20146.178 7.612 7.081 1.00 0.00 C **ATOM** 238 CG1 VAL A 20147.289 6.984 7.908 1.00 0.00 C **ATOM** 239 CG2 VALA 20146.748 8.330 5.868 1.00 0.00 C **ATOM** 240 H VALA 20144.237 8.041 5.462 1.00 0.00 H **ATOM** 241 HA VALA 20145.687 5.753 6.139 1.00 0.00 H **ATOM** 242 HB VALA 20145.670 8.340 7.697 1.00 0.00 H **ATOM** 243 1HG1 VAL A 20146.955 6.867 8.929 1.00 0.00 H **ATOM** 244 2HG1 VAL A 20148.160 7.622 7.885 1.00 0.00 H **ATOM** 245 3HG1 VAL A 20147.539 6.017 7.499 1.00 0.00 H **ATOM ATOM** 246 1HG2 VAL A 20147.025 7.605 5.117 1.00 0.00 H 247 2HG2 VAL A 20147.620 8.896 6.161 1.00 0.00 H ATOM 248 3HG2 VAL A 20146.004 9.001 5.463 1.00 0.00 H **ATOM** 249 N GLY A 21144.928 4.797 8.312 1.00 0.00 N **ATOM** 250 CA GLY A 21144.352 4.163 9.482 1.00 0.00 C **ATOM** 251 C GLY A 21143,278 3.154 9.125 1.00 0.00 C ATOM **ATOM** 252 O GLYA 21143.175 2.098 9.750 1.00 0.00 O ATOM 253 H GLY A 21145.658 4.358 7.827 1.00 0.00 H

254 1HA GLY A 21145.137 3.658 10.028 1.00 0.00 H ATOM 255 2HA GLY A 21143.920 4.923 10.116 1.00 0.00 H ATOM 256 N SER A 22142.474 3.480 8.118 1.00 0.00 N ATOM 257 CA SER A 22141.402 2.595 7.678 1.00 0.00 C 258 C SER A 22141.949 1.470 6.805 1.00 0.00 C ATOM 259 O SER A 22142.939 1.645 6.095 1.00 0.00 O ATOM ATOM 260 CB SER A 22140.344 3.385 6.907 1.00 0.00 C 261 OG SER A 22140.269 4.723 7.368 1.00 0.00 O ATOM **ATOM** 262 H SER A 22142.606 4.335 7.659 1.00 0.00 H 263 HA SER A 22140.947 2.164 8.556 1.00 0.00 H ATOM 264 1HB SER A 22140.598 3.395 5.857 1.00 0.00 H ATOM 265 2HB SER A 22139.380 2.916 7.039 1.00 0.00 H ATOM 266 HG SER A 22140.281 4.731 8.329 1.00 0.00 H ATOM 267 N LEUA 23141.298 0.312 6.864 1.00 0.00 N ATOM 268 CA LEU A 23141.719 -0.842 6.079 1.00 0.00 C **ATOM** 269 C LEUA 23141.156 -0.772 4.664 1.00 0.00 C ATOM 270 O LEUA 23140.073 -0.229 4.441 1.00 0.00 O 271 CB LEU A 23141.267 -2.138 6.756 1.00 0.00 C **ATOM** 272 CG LEU A 23141.762 -2.325 8.192 1.00 0.00 C ATOM 273 CD1 LEU A 23140.763 -3.143 8.997 1.00 0.00 C ATOM 274 CD2 LEU A 23143.129 -2.990 8.201 1.00 0.00 C ATOM 275 H LEUA 23140.515 0.233 7.449 1.00 0.00 H ATOM 276 HA LEU A 23142.797 -0.831 6.026 1.00 0.00 H **ATOM ATOM** 277 1HB LEU A 23140.186 -2.158 6.763 1.00 0.00 H 278 2HB LEU A 23141.622 -2.970 6.167 1.00 0.00 H **ATOM** 279 HG LEU A 23141.855 -1.357 8.662 1.00 0.00 H **ATOM** 280 1HD1 LEU A 23140.721 -2.765 10.008 1.00 0.00 H ATOM 281 2HD1 LEU A 23141.074 -4.177 9.012 1.00 0.00 H ATOM 282 3HD1 LEU A 23139.786 -3.066 8.544 1.00 0.00 H ATOM 283 1HD2 LEU A 23143.718 -2.591 9.013 1.00 0.00 H ATOM ATOM 284 2HD2 LEU A 23143.630 -2.796 7.264 1.00 0.00 H

- ATOM 285 3HD2 LEU A 23143.010 -4.056 8.332 1.00 0.00 H
- ATOM 286 N ALA A 24141.896 -1.326 3.709 1.00 0.00 N
- ATOM 287 CA ALA A 24141.472 -1.326 2.314 1.00 0.00 C
- ATOM 288 C ALA A 24142.116 -2.474 1.545 1.00 0.00 C
- ATOM 289 O ALA A 24143.252 -2.858 1.820 1.00 0.00 O
- ATOM 290 CB ALA A 24141.806 0.005 1.660 1.00 0.00 C
- ATOM 291 H ALA A 24142.750 -1.744 3.949 1.00 0.00 H
- ATOM 292 HA ALA A 24140.398 -1.451 2.294 1.00 0.00 H
- ATOM 293 1HB ALA A 24142.746 -0.079 1.134 1.00 0.00 H
- ATOM 294 2HB ALA A 24141.884 0.770 2.419 1.00 0.00 H
- ATOM 295 3HB ALA A 24141.026 0.270 0.962 1.00 0.00 H
- ATOM 296 N GLUA 25141.383 -3.016 0.578 1.00 0.00 N
- ATOM 297 CA GLU A 25141.883 -4.121 -0.233 1.00 0.00 C
- ATOM 298 C GLU A 25142.149 -3.669 -1.665 1.00 0.00 C
- ATOM 299 O GLUA 25141.544 -2.711 -2.146 1.00 0.00 O
- ATOM 300 CB GLU A 25140.883 -5.278 -0.229 1.00 0.00 C
- ATOM 301 CG GLUA 25141.402 -6.533 -0.912 1.00 0.00 C
- ATOM 302 CD GLUA 25140.359 -7.631 -0.983 1.00 0.00 C
- ATOM 303 OE1 GLU A 25140.483 -8.511 -1.860 1.00 0.00 O
- ATOM 304 OE2 GLU A 25139.420 -7.612 -0.159 1.00 0.00 O
- ATOM 305 H GLUA 25140.484 -2.666 0.406 1.00 0.00 H
- ATOM 306 HA GLUA 25142.812 -4.458 0.203 1.00 0.00 H
- ATOM 307 1HB GLU A 25140.640 -5.526 0.794 1.00 0.00 H
- ATOM 308 2HB GLU A 25139.984 -4.963 -0.738 1.00 0.00 H
- ATOM 309 1HG GLU A 25141.704 -6.281 -1.917 1.00 0.00 H
- ATOM 310 2HG GLU A 25142.255 -6.900 -0.362 1.00 0.00 H
- ATOM 311 N VALA 26143.058 -4.363 -2.340 1.00 0.00 N
- ATOM 312 CA VALA 26143.405 -4.034 -3.718 1.00 0.00 C
- ATOM 313 C VALA 26143.016 -5.163 -4.667 1.00 0.00 C
- ATOM 314 O VALA 26142.958 -6.327 -4.272 1.00 0.00 O
- ATOM 315 CB VAL A 26144.911 -3.750 -3.867 1.00 0.00 C

- ATOM 316 CG1 VAL A 26145.220 -3.217 -5.257 1.00 0.00 C
- ATOM 317 CG2 VAL A 26145.378 -2.775 -2.798 1.00 0.00 C
- ATOM 318 H VALA 26143.507 -5.116 -1.903 1.00 0.00 H
- ATOM 319 HA VALA 26142.862 -3.141 -3.995 1.00 0.00 H
- ATOM 320 HB VALA 26145.446 -4.679 -3.735 1.00 0.00 H
- ATOM 321 1HG1 VAL A 26146.167 -2.698 -5.241 1.00 0.00 H
- ATOM 322 2HG1 VAL A 26144.441 -2.535 -5.563 1.00 0.00 H
- ATOM 323 3HG1 VAL A 26145.272 -4.039 -5.955 1.00 0.00 H
- ATOM 324 1HG2 VAL A 26144.985 -3.076 -1.838 1.00 0.00 H
- ATOM 325 2HG2 VAL A 26145.026 -1.782 -3.036 1.00 0.00 H
- ATOM 326 3HG2 VAL A 26146.458 -2.773 -2.759 1.00 0.00 H
- ATOM 327 N LYS A 27142.751 -4.810 -5.921 1.00 0.00 N
- ATOM 328 CA LYS A 27142.369 -5.793 -6.927 1.00 0.00 C
- ATOM 329 C LYS A 27143.583 -6.248 -7.731 1.00 0.00 C
- ATOM 330 O LYS A 27144.100 -5.507 -8.567 1.00 0.00 O
- ATOM 331 CB LYS A 27141.311 -5.209 -7.865 1.00 0.00 C
- ATOM 332 CG LYS A 27140.596 -6.257 -8.703 1.00 0.00 C
- ATOM 333 CD LYS A 27139.384 -5.672 -9.410 1.00 0.00 C
- ATOM 334 CE LYS A 27139.017 -6.478 -10.646 1.00 0.00 C
- ATOM 335 NZ LYS A 27137.542 -6.568 -10.832 1.00 0.00 N
- ATOM 336 H LYS A 27142.815 -3.865 -6.176 1.00 0.00 H
- ATOM 337 HA LYS A 27141.951 -6.647 -6.414 1.00 0.00 H
- ATOM 338 1HB LYS A 27140.573 -4.686 -7.276 1.00 0.00 H
- ATOM 339 2HB LYS A 27141.787 -4.509 -8.535 1.00 0.00 H
- ATOM 340 1HG LYS A 27141.280 -6.641 -9.443 1.00 0.00 H
- ATOM 341 2HG LYS A 27140.271 -7.060 -8.057 1.00 0.00 H
- ATOM 342 1HD LYS A 27138.545 -5.673 -8.729 1.00 0.00 H
- ATOM 343 2HD LYS A 27139.607 -4.657 -9.707 1.00 0.00 H
- ATOM 344 1HE LYS A 27139.452 -6.003 -11.512 1.00 0.00 H
- ATOM 345 2HE LYS A 27139.419 -7.475 -10.542 1.00 0.00 H
- ATOM 346 1HZ LYS A 27137.058 -6.447 -9.919 1.00 0.00 H

- ATOM 347 2HZ LYS A 27137.287 -7.496 -11.226 1.00 0.00 H
- ATOM 348 3HZ LYS A 27137.218 -5.825 -11.485 1.00 0.00 H
- ATOM 349 N GLU A 28144.031 -7.473 -7.475 1.00 0.00 N
- ATOM 350 CA GLU A 28145.184 -8.026 -8.174 1.00 0.00 C
- ATOM 351 C GLU A 28145.135 -9.551 -8.180 1.00 0.00 C
- ATOM 352 O GLU A 28144.125 -10.152 -7.814 1.00 0.00 O
- ATOM 353 CB GLU A 28146.483 -7.545 -7.523 1.00 0.00 C
- ATOM 354 CG GLU A 28147.503 -7.017 -8.517 1.00 0.00 C
- ATOM 355 CD GLU A 28148.752 -7.873 -8.585 1.00 0.00 C
- ATOM 356 OE1 GLU A 28149.528 -7.872 -7.606 1.00 0.00 O
- ATOM 357 OE2 GLU A 28148.955 -8.548 -9.617 1.00 0.00 O
- ATOM 358 H GLUA 28143.576 -8.016 -6.798 1.00 0.00 H
- ATOM 359 HA GLU A 28145.152 -7.674 -9.194 1.00 0.00 H
- ATOM 360 1HB GLU A 28146.249 -6.755 -6.824 1.00 0.00 H
- ATOM 361 2HB GLU A 28146.929 -8.368 -6.983 1.00 0.00 H
- ATOM 362 1HG GLU A 28147.052 -6.989 -9.497 1.00 0.00 H
- ATOM 363 2HG GLU A 28147.786 -6.016 -8.224 1.00 0.00 H
- ATOM 364 N ASNA 29146.234 -10.172 -8.599 1.00 0.00 N
- ATOM 365 CA ASN A 29146.317 -11.626 -8.650 1.00 0.00 C
- ATOM 366 C ASN A 29146.467 -12.213 -7.249 1.00 0.00 C
- ATOM 367 O ASN A 29145.645 -13.020 -6.814 1.00 0.00 O
- ATOM 368 CB ASN A 29147.493 -12.059 -9.529 1.00 0.00 C
- ATOM 369 CG ASN A 29147.063 -12.398 -10.943 1.00 0.00 C
- ATOM 370 OD1 ASN A 29146.874 -13.566 -11.284 1.00 0.00 O
- ATOM 371 ND2 ASN A 29146.907 -11.375 -11.776 1.00 0.00 N
- ATOM 372 H ASN A 29147.008 -9.638 -8.876 1.00 0.00 H
- ATOM 373 HA ASN A 29145.400 -11.995 -9.085 1.00 0.00 H
- ATOM 374 1HB ASN A 29148.214 -11.257 -9.576 1.00 0.00 H
- ATOM 375 2HB ASN A 29147.958 -12.932 -9.095 1.00 0.00 H
- ATOM 376 1HD2 ASN A 29147.076 -10.472 -11.435 1.00 0.00 H
- ATOM 377 2HD2 ASN A 29146.629 -11.566 -12.696 1.00 0.00 H

ATOM 378 N PRO A 30147.526 -11.816 -6.522 1.00 0.00 N 379 CA PRO A 30147.782 -12.306 -5.166 1.00 0.00 C ATOM 380 C PRO A 30146.884 -11.635 -4.126 1.00 0.00 C ATOM 381 O PRO A 30147.049 -10.453 -3.828 1.00 0.00 O **ATOM** 382 CB PRO A 30149.243 -11.926 -4.932 1.00 0.00 C ATOM ATOM 383 CG PRO A 30149.448 -10.704 -5.760 1.00 0.00 C 384 CD PRO A 30148.557 -10.856 -6.965 1.00 0.00 C ATOM 385 HA PRO A 30147.671 -13.378 -5.105 1.00 0.00 H ATOM 386 1HB PRO A 30149.403 -11.727 -3.883 1.00 0.00 H ATOM ATOM 387 2HB PRO A 30149.884 -12.733 -5.255 1.00 0.00 H **ATOM** 388 1HG PRO A 30149.166 -9.829 -5.194 1.00 0.00 H 389 2HG PRO A 30150.482 -10.638 -6.064 1.00 0.00 H ATOM 390 1HD PRO A 30148.113 -9.908 -7.225 1.00 0.00 H ATOM 391 2HD PRO A 30149.117 -11.252 -7.799 1.00 0.00 H ATOM 392 N PRO A 31145.919 -12.382 -3.559 1.00 0.00 N ATOM ATOM 393 CA PRO A 31145.001 -11.844 -2.550 1.00 0.00 C 394 C PRO A 31145.700 -11.555 -1.226 1.00 0.00 C ATOM 395 O PRO A 31146.226 -12.461 -0.579 1.00 0.00 O ATOM 396 CB PRO A 31143.968 -12.960 -2.376 1.00 0.00 C ATOM 397 CG PRO A 31144.686 -14.204 -2.768 1.00 0.00 C **ATOM** 398 CD PRO A 31145.648 -13.802 -3.851 1.00 0.00 C ATOM **ATOM** 399 HA PRO A 31144.511 -10.946 -2.899 1.00 0.00 H 400 1HB PRO A 31143.644 -12.996 -1.346 1.00 0.00 H ATOM 401 2HB PRO A 31143.121 -12.775 -3.019 1.00 0.00 H ATOM 402 1HG PRO A 31145.224 -14.600 -1.918 1.00 0.00 H ATOM 403 2HG PRO A 31143.982 -14.932 -3.142 1.00 0.00 H ATOM ATOM 404 1HD PRO A 31146.553 -14.388 -3.790 1.00 0.00 H ATOM 405 2HD PRO A 31145.189 -13.914 -4.822 1.00 0.00 H 406 N PHE A 32145.703 -10.287 -0.828 1.00 0.00 N ATOM 407 CA PHE A 32146.338 -9.878 0.420 1.00 0.00 C **ATOM** ATOM 408 C PHE A 32145.479 -8.858 1.160 1.00 0.00 C

409 O PHE A 32144.591 -8.238 0.574 1.00 0.00 O **ATOM** 410 CB, PHE A 32147.723 -9.291 0.142 1.00 0.00 C ATOM **ATOM** 411 CG PHE A 32147.736 -8.287 -0.975 1.00 0.00 C ATOM 412 CD1 PHE A 32148.424 -8.547 -2.150 1.00 0.00 C 413 CD2 PHE A 32147.060 -7.083 -0.851 1.00 0.00 C ATOM ATOM 414 CE1 PHE A 32148.438 -7.626 -3.180 1.00 0.00 C 415 CE2 PHE A 32147.070 -6.158 -1.878 1.00 0.00 C 416 CZ PHE A 32147.760 -6.429 -3.044 1.00 0.00 C **ATOM** 417 H PHE A 32145.267 -9.610 -1.386 1.00 0.00 H ATOM 418 HA PHE A 32146.447 -10.756 1.038 1.00 0.00 H ATOM 419 1HB PHE A 32148.083 -8.799 1.033 1.00 0.00 H ATOM 420 2HB PHE A 32148.399 -10.090 -0.120 1.00 0.00 H ATOM ATOM 421 HD1 PHE A 32148.955 -9.482 -2.257 1.00 0.00 H ATOM 422 HD2 PHE A 32146.521 -6.871 0.060 1.00 0.00 H 423 HE1 PHE A 32148.978 -7.839 -4.090 1.00 0.00 H ATOM 424 HE2 PHE A 32146.540 -5.224 -1.769 1.00 0.00 H ATOM 425 HZ PHE A 32147.770 -5.708 -3.847 1.00 0.00 H ATOM 426 N TYR A 33145.750 -8.690 2.450 1.00 0.00 N ATOM 427 CA TYR A 33145.001 -7.746 3.272 1.00 0.00 C ATOM **ATOM** 428 C TYR A 33145.945 -6.812 4.022 1.00 0.00 C 429 O TYR A 33146.943 -7.251 4.594 1.00 0.00 O ATOM 430 CB TYR A 33144.109 -8.494 4.264 1.00 0.00 C ATOM 431 CG TYR A 33142.774 -8.908 3.687 1.00 0.00 C **ATOM** ATOM 432 CD1 TYR A 33142.316 -10.213 3.813 1.00 0.00 C 433 CD2 TYR A 33141.973 -7.993 3.014 1.00 0.00 C ATOM 434 CE1 TYR A 33141.097 -10.594 3.287 1.00 0.00 C **ATOM** ATOM 435 CE2 TYR A 33140.752 -8.368 2.486 1.00 0.00 C 436 CZ TYR A 33140.319 -9.668 2.625 1.00 0.00 C **ATOM** 437 OH TYR A 33139.104 -10.045 2.099 1.00 0.00 O ATOM **ATOM** 438 H TYR A 33146.469 -9.214 2.860 1.00 0.00 H ATOM 439 HA TYR A 33144.379 -7.156 2.615 1.00 0.00 H

440 1HB TYR A 33144.620 -9.387 4.592 1.00 0.00 H **ATOM** 441 2HB TYR A 33143.921 -7.859 5.117 1.00 0.00 H 442 HD1 TYR A 33142.927 -10.935 4.333 1.00 0.00 H ATOM ATOM 443 HD2 TYR A 33142.316 -6.975 2.907 1.00 0.00 H 444 HE1 TYR A 33140.757 -11.614 3.396 1.00 0.00 H ATOM ATOM 445 HE2 TYR A 33140.144 -7.642 1.967 1.00 0.00 H 446 HH TYR A 33138.462 -10.131 2.807 1.00 0.00 H ATOM 447 N GLY A 34145.623 -5.522 4.016 1.00 0.00 N ATOM 448 CA GLY A 34146.453 -4.548 4.700 1.00 0.00 C ATOM 449 C GLY A 34145.682 -3.302 5.091 1.00 0.00 C ATOM 450 O GLY A 34144.454 -3.272 5.009 1.00 0.00 O ATOM 451 H GLY A 34144.817 -5.230 3.543 1.00 0.00 H **ATOM** ATOM 452 1HA GLY A 34146.861 -5.001 5.591 1.00 0.00 H 453 2HA GLY A 34147.267 -4.264 4.049 1.00 0.00 H ATOM 454 N VALA 35146.405 -2.272 5.520 1.00 0.00 N ATOM 455 CA VALA 35145.783 -1.018 5.927 1.00 0.00 C ATOM 456 C VALA 35146.505 0.177 5.313 1.00 0.00 C ATOM 457 O VALA 35147.721 0.150 5.125 1.00 0.00 O ATOM 458 CB VALA 35145.769 -0.870 7.462 1.00 0.00 C ATOM 459 CG1 VAL A 35147.188 -0.848 8.012 1.00 0.00 C ATOM 460 CG2 VAL A 35145.010 0.383 7.873 1.00 0.00 C ATOM 461 H VALA 35147.380 -2.359 5.565 1.00 0.00 H **ATOM** 462 HA VALA 35144.760 -1.026 5.579 1.00 0.00 H **ATOM** 463 HB VALA 35145.261 -1.726 7.880 1.00 0.00 H ATOM 464 1HG1 VAL A 35147.862 -1.287 7.291 1.00 0.00 H ATOM 465 2HG1 VAL A 35147.226 -1.413 8.931 1.00 0.00 H **ATOM** 466 3HG1 VAL A 35147.483 0.173 8.204 1.00 0.00 H ATOM 467 1HG2 VAL A 35143.960 0.255 7.654 1.00 0.00 H **ATOM** 468 2HG2 VAL A 35145.392 1.231 7.324 1.00 0.00 H ATOM 469 3HG2 VAL A 35145.140 0.551 8.931 1.00 0.00 H ATOM ATOM 470 N ILE A 36145.747 1.224 5.003 1.00 0.00 N

471 CA ILE A 36146.316 2.429 4.411 1.00 0.00 C 472 C ILE A 36147.242 3.136 5.395 1.00 0.00 C **ATOM** ATOM 473 O ILEA 36146.961 3.200 6.592 1.00 0.00 O 474 CB ILE A 36145.216 3.410 3.960 1.00 0.00 C 475 CG1 ILE A 36144.192 2.693 3.078 1.00 0.00 C ATOM 476 CG2 ILE A 36145.828 4.590 3.218 1.00 0.00 C **ATOM** ATOM 477 CD1 ILE A 36143.055 3.584 2.627 1.00 0.00 C 478 H ILE A 36144.783 1.186 5.177 1.00 0.00 H ATOM 479 HA ILE A 36146.887 2.136 3.542 1.00 0.00 H **ATOM** 480 HB ILE A 36144.720 3.789 4.841 1.00 0.00 H ATOM 481 1HG1 ILE A 36144.686 2.316 2.196 1.00 0.00 H ATOM ATOM 482 2HG1 ILE A 36143.767 1.866 3.629 1.00 0.00 H 483 1HG2 ILE A 36146.782 4.299 2.805 1.00 0.00 H **ATOM** 484 2HG2 ILE A 36145.968 5.413 3.903 1.00 0.00 H ATOM 485 3HG2 ILE A 36145.168 4.894 2.420 1.00 0.00 H **ATOM** 486 1HD1 ILE A 36143.454 4.434 2.094 1.00 0.00 H **ATOM** 487 2HD1 ILE A 36142.502 3.928 3.489 1.00 0.00 H **ATOM** 488 3HD1 ILE A 36142.397 3.027 1.976 1.00 0.00 H ATOM 489 N ARGA 37148.348 3.667 4.882 1.00 0.00 N ATOM 490 CA ARG A 37149.317 4.368 5.718 1.00 0.00 C **ATOM** 491 C ARGA 37149.519 5.800 5.231 1.00 0.00 C **ATOM** 492 O ARGA 37149.161 6.756 5.921 1.00 0.00 O **ATOM** 493 CB ARG A 37150.653 3.625 5.718 1.00 0.00 C **ATOM** 494 CG ARG A 37150.520 2.138 6.004 1.00 0.00 C **ATOM** 495 CD ARG A 37150.448 1.861 7.496 1.00 0.00 C **ATOM** 496 NE ARG A 37149.225 2.391 8.094 1.00 0.00 N **ATOM** 497 CZ ARG A 37149.068 2.601 9.399 1.00 0.00 C ATOM 498 NH1 ARG A 37150.053 2.328 10.246 1.00 0.00 N **ATOM** 499 NH2 ARG A 37147.924 3.087 9.859 1.00 0.00 N ATOM 500 H ARG A 37148.518 3.582 3.922 1.00 0.00 H **ATOM** 501 HA ARG A 37148.929 4.395 6.724 1.00 0.00 H ATOM

502 1HB ARG A 37151.119 3.744 4.752 1.00 0.00 H ATOM 503 2HB ARG A 37151.293 4.058 6.473 1.00 0.00 H ATOM 504 1HG ARG A 37149.620 1.770 5.536 1.00 0.00 H **ATOM** 505 2HG ARG A 37151.376 1.624 5.592 1.00 0.00 H **ATOM** 506 1HD ARG A 37150.480 0.793 7.654 1.00 0.00 H **ATOM** ATOM 507 2HD ARG A 37151.301 2.320 7.976 1.00 0.00 H 508 HE ARG A 37148.481 2.601 7.491 1.00 0.00 H ATOM 509 1HH1 ARG A 37150.918 1.961 9.906 1.00 0.00 H ATOM 510 2HH1 ARG A 37149.929 2.488 11.224 1.00 0.00 H ATOM 511 1HH2 ARG A 37147.178 3.295 9.226 1.00 0.00 H **ATOM** 512 2HH2 ARG A 37147.805 3.245 10.839 1.00 0.00 H ATOM 513 N TRP A 38150.092 5.942 4.041 1.00 0.00 N ATOM 514 CA TRPA 38150.340 7.259 3.465 1.00 0.00 C ATOM 515 C TRPA 38149.621 7.414 2.128 1.00 0.00 C **ATOM** 516 O TRPA 38149.714 6.549 1.257 1.00 0.00 O **ATOM** 517 CB TRP A 38151.845 7.487 3.282 1.00 0.00 C **ATOM** 518 CG TRP A 38152.172 8.692 2.450 1.00 0.00 C **ATOM** 519 CD1 TRP A 38152.385 9.965 2.896 1.00 0.00 C **ATOM** 520 CD2 TRP A 38152.315 8.736 1.025 1.00 0.00 C **ATOM** 521 NE1 TRP A 38152.652 10.798 1.836 1.00 0.00 N ATOM 522 CE2 TRP A 38152.614 10.067 0.677 1.00 0.00 C ATOM 523 CE3 TRP A 38152.218 7.779 0.011 1.00 0.00 C **ATOM** 524 CZ2 TRP A 38152.818 10.462 -0.644 1.00 0.00 C ATOM 525 CZ3 TRP A 38152.421 8.174 -1.298 1.00 0.00 C **ATOM** 526 CH2 TRP A 38152.718 9.504 -1.616 1.00 0.00 C ATOM 527 H TRPA 38150.355 5.143 3.538 1.00 0.00 H **ATOM** 528 HA TRP A 38149.956 7.998 4.152 1.00 0.00 H **ATOM** 529 1HB TRP A 38152.303 7.619 4.251 1.00 0.00 H ATOM 530 2HB TRP A 38152.276 6.622 2.800 1.00 0.00 H ATOM 531 HD1 TRP A 38152.347 10.260 3.934 1.00 0.00 H ATOM 532 HE1 TRP A 38152.840 11.757 1.898 1.00 0.00 H

533 HE3 TRP A 38151.989 6.750 0.236 1.00 0.00 H ATOM 534 HZ2 TRP A 38153.045 11.485 -0.905 1.00 0.00 H 535 HZ3 TRP A 38152.350 7.447 -2.094 1.00 0.00 H ATOM **ATOM** 536 HH2 TRP A 38152.868 9.767 -2.653 1.00 0.00 H 537 N ILE A 39148.914 8.527 1.971 1.00 0.00 N ATOM 538 CA ILE A 39148.186 8.807 0.740 1.00 0.00 C ATOM 539 C ILE A 39148.655 10.121 0.126 1.00 0.00 C ATOM 540 O ILE A 39148.335 11.200 0.627 1.00 0.00 O ATOM 541 CB ILE A 39146.667 8.879 0.986 1.00 0.00 C **ATOM** 542 CG1 ILE A 39146.190 7.640 1.748 1.00 0.00 C **ATOM** 543 CG2 ILE A 39145.921 9.014 -0.333 1.00 0.00 C **ATOM** 544 CD1 ILE A 39145.160 7.947 2.814 1.00 0.00 C ATOM **ATOM** 545 H ILE A 39148.886 9.181 2.700 1.00 0.00 H 546 HA ILE A 39148.383 8.004 0.044 1.00 0.00 H ATOM 547 HB ILE A 39146.462 9.757 1.578 1.00 0.00 H **ATOM** 548 1HG1 ILE A 39145.747 6.945 1.051 1.00 0.00 H ATOM 549 2HG1 ILE A 39147.036 7.172 2.228 1.00 0.00 H ATOM 550 1HG2 ILE A 39146.587 9.412 -1.085 1.00 0.00 H **ATOM** 551 2HG2 ILE A 39145.082 9.681 -0.206 1.00 0.00 H **ATOM** 552 3HG2 ILE A 39145.564 8.044 -0.647 1.00 0.00 H ATOM 553 1HD1 ILE A 39145.546 8.705 3.479 1.00 0.00 H **ATOM** 554 2HD1 ILE A 39144.946 7.049 3.377 1.00 0.00 H ATOM 555 3HD1 ILE A 39144.254 8.303 2.348 1.00 0.00 H ATOM **ATOM** 556 N GLY A 40149.421 10.027 -0.956 1.00 0.00 N 557 CA GLY A 40149.925 11.219 -1.610 1.00 0.00 C **ATOM** 558 C GLY A 40150.479 10.940 -2.992 1.00 0.00 C **ATOM** 559 O GLY A 40150.290 9.853 -3.539 1.00 0.00 O **ATOM** 560 H GLY A 40149.648 9.142 -1.310 1.00 0.00 H ATOM 561 1HA GLY A 40149.122 11.936 -1.694 1.00 0.00 H **ATOM** 562 2HA GLY A 40150.707 11.646 -1.001 1.00 0.00 H ATOM 563 N GLNA 41151.164 11.928 -3.558 1.00 0.00 N

564 CA GLN A 41151.749 11.795 -4.885 1.00 0.00 C **ATOM ATOM** 565 C GLN A 41153.233 12.162 -4.861 1.00 0.00 C 566 O GLNA 41153.589 13.310 -4.593 1.00 0.00 O **ATOM** 567 CB GLN A 41151.006 12.692 -5.874 1.00 0.00 C **ATOM** 568 CG GLN A 41149.494 12.552 -5.804 1.00 0.00 C **ATOM** 569 CD GLN A 41148.780 13.884 -5.930 1.00 0.00 C **ATOM** 570 OE1 GLN A 41148.762 14.682 -4.993 1.00 0.00 O **ATOM ATOM** 571 NE2 GLN A 41148.187 14.129 -7.091 1.00 0.00 N **ATOM** 572 H GLNA 41151.277 12.770 -3.071 1.00 0.00 H **ATOM** 573 HA GLN A 41151.645 10.767 -5.196 1.00 0.00 H 574 1HB GLN A 41151.260 13.721 -5.669 1.00 0.00 H **ATOM** 575 2HB GLN A 41151.324 12.446 -6.875 1.00 0.00 H **ATOM** 576 1HG GLN A 41149.166 11.910 -6.606 1.00 0.00 H ATOM 577 2HG GLN A 41149.230 12.107 -4.856 1.00 0.00 H ATOM 578 1HE2 GLN A 41148.242 13.447 -7.792 1.00 0.00 H ATOM 579 2HE2 GLN A 41147.718 14.983 -7.200 1.00 0.00 H ATOM 580 N PRO A 42154.123 11.192 -5.140 1.00 0.00 N **ATOM** ATOM 581 CA PRO A 42155.571 11.431 -5.144 1.00 0.00 C 582 C PRO A 42155.970 12.538 -6.115 1.00 0.00 C ATOM 583 O PRO A 42155.226 12.862 -7.040 1.00 0.00 O **ATOM** 584 CB PRO A 42156.160 10.089 -5.592 1.00 0.00 C ATOM 585 CG PRO A 42155.105 9.086 -5.277 1.00 0.00 C ATOM 586 CD PRO A 42153.796 9.795 -5.471 1.00 0.00 C ATOM 587 HA PRO A 42155.932 11.675 -4.156 1.00 0.00 H **ATOM** 588 1HB PRO A 42156.372 10.122 -6.650 1.00 0.00 H **ATOM** 589 2HB PRO A 42157.068 9.891 -5.043 1.00 0.00 H **ATOM** 590 1HG PRO A 42155.182 8.247 -5.953 1.00 0.00 H ATOM 591 2HG PRO A 42155.204 8.755 -4.253 1.00 0.00 H **ATOM** 592 1HD PRO A 42153.468 9.707 -6.496 1.00 0.00 H ATOM 593 2HD PRO A 42153.049 9.403 -4.796 1.00 0.00 H ATOM 594 N PRO A 43157.157 13.135 -5.916 1.00 0.00 N ATOM

595 CA PRO A 43157.653 14.210 -6.779 1.00 0.00 C 596 C PRO A 43158.072 13.701 -8.154 1.00 0.00 C ATOM 597 O PRO A 43159.237 13.372 -8.377 1.00 0.00 O ATOM 598 CB PRO A 43158.867 14.743 -6.019 1.00 0.00 C ATOM 599 CG PRO A 43159.338 13.593 -5.199 1.00 0.00 C ATOM 600 CD PRO A 43158.107 12.807 -4.836 1.00 0.00 C **ATOM** ATOM 601 HA PRO A 43156.922 14.995 -6.894 1.00 0.00 H 602 1HB PRO A 43159.621 15.063 -6.722 1.00 0.00 H **ATOM** 603 2HB PRO A 43158.570 15.575 -5.398 1.00 0.00 H **ATOM** 604 1HG PRO A 43160.015 12.982 -5.778 1.00 0.00 H ATOM 605 2HG PRO A 43159.827 13.954 -4.306 1.00 0.00 H ATOM ATOM 606 1HD PRO A 43158.325 11.749 -4.822 1.00 0.00 H 607 2HD PRO A 43157.724 13.126 -3.877 1.00 0.00 H ATOM 608 N GLY A 44157.115 13.641 -9.073 1.00 0.00 N ATOM ATOM 609 CA GLY A 44157.408 13.172 -10.414 1.00 0.00 C 610 C GLY A 44156.177 12.664 -11.134 1.00 0.00 C ATOM 611 O GLY A 44155.900 13.064 -12.265 1.00 0.00 O **ATOM** 612 H GLY A 44156.204 13.916 -8.839 1.00 0.00 H ATOM 613 1HA GLY A 44157.832 13.986 -10.982 1.00 0.00 H ATOM 614 2HA GLY A 44158.132 12.374 -10.354 1.00 0.00 H ATOM 615 N LEUA 45155.434 11.777 -10.479 1.00 0.00 N ATOM 616 CA LEU A 45154.226 11.214 -11.068 1.00 0.00 C **ATOM** 617 C LEUA 45153.012 11.507 -10.196 1.00 0.00 C **ATOM** 618 O LEUA 45152.895 10.989 -9.086 1.00 0.00 O ATOM 619 CB LEU A 45154.382 9.704 -11.255 1.00 0.00 C ATOM 620 CG LEU A 45154.896 8.948 -10.027 1.00 0.00 C ATOM 621 CD1 LEU A 45154.503 7.479 -10.098 1.00 0.00 C ATOM 622 CD2 LEU A 45156.407 9.097 -9.903 1.00 0.00 C ATOM 623 H LEUA 45155.705 11.497 -9.578 1.00 0.00 H ATOM 624 HA LEU A 45154.080 11.674 -12.034 1.00 0.00 H ATOM ATOM 625 1HB LEU A 45153.420 9.294 -11.528 1.00 0.00 H

626 2HB LEU A 45155.071 9.532 -12.069 1.00 0.00 H ATOM 627 HG LEU A 45154.444 9.371 -9.141 1.00 0.00 H 628 1HD1 LEU A 45153.934 7.217 -9.218 1.00 0.00 H **ATOM ATOM** 629 2HD1 LEU A 45155.393 6.869 -10.146 1.00 0.00 H 630 3HD1 LEU A 45153.903 7.308 -10.979 1.00 0.00 H ATOM 631 1HD2 LEU A 45156.882 8.155 -10.133 1.00 0.00 H ATOM 632 2HD2 LEU A 45156.657 9.388 -8.893 1.00 0.00 H **ATOM** 633 3HD2 LEU A 45156.754 9.853 -10.591 1.00 0.00 H **ATOM** 634 N ASNA 46152.106 12.339 -10.702 1.00 0.00 N **ATOM** 635 CA ASN A 46150.905 12.688 -9.956 1.00 0.00 C **ATOM** 636 C ASN A 46149.929 11.517 -9.931 1.00 0.00 C **ATOM** 637 O ASN A 46149.305 11.193 -10.942 1.00 0.00 O **ATOM** 638 CB ASN A 46150.233 13.914 -10.577 1.00 0.00 C **ATOM** 639 CG ASN A 46149.461 14.730 -9.558 1.00 0.00 C **ATOM** 640 OD1 ASN A 46150.024 15.208 -8.573 1.00 0.00 O ATOM 641 ND2 ASN A 46148.164 14.891 -9.790 1.00 0.00 N ATOM 642 H ASN A 46152.249 12.722 -11.592 1.00 0.00 H **ATOM** 643 HA ASN A 46151.197 12.921 -8.943 1.00 0.00 H ATOM 644 1HB ASN A 46150.990 14.547 -11.017 1.00 0.00 H **ATOM** 645 2HB ASN A 46149.548 13.590 -11.346 1.00 0.00 H ATOM 646 1HD2 ASN A 46147.782 14.480 -10.594 1.00 0.00 H **ATOM** 647 2HD2 ASN A 46147.640 15.414 -9.148 1.00 0.00 H ATOM 648 N GLUA 47149.803 10.889 -8.768 1.00 0.00 N **ATOM** 649 CA GLUA 47148.906 9.754 -8.603 1.00 0.00 C ATOM 650 C GLUA 47148.706 9.434 -7.126 1.00 0.00 C **ATOM** 651 O GLUA 47149.665 9.143 -6.412 1.00 0.00 O **ATOM** 652 CB GLUA 47149.452 8.526 -9.334 1.00 0.00 C **ATOM** 653 CG GLU A 47150.963 8.373 -9.232 1.00 0.00 C ATOM 654 CD GLUA 47151.518 7.390 -10.243 1.00 0.00 C **ATOM** 655 OE1 GLU A 47151.557 7.732 -11.444 1.00 0.00 O **ATOM** 656 OE2 GLU A 47151.914 6.278 -9.835 1.00 0.00 O

657 H GLUA 47150.329 11.196 -8.002 1.00 0.00 H 658 HA GLU A 47147.951 10.022 -9.033 1.00 0.00 H ATOM 659 1HB GLU A 47148.996 7.640 -8.917 1.00 0.00 H **ATOM ATOM** 660 2HB GLU A 47149.189 8.596 -10.379 1.00 0.00 H 661 1HG GLU A 47151.419 9.337 -9.401 1.00 0.00 H ATOM **ATOM** 662 2HG GLU A 47151.213 8.027 -8.240 1.00 0.00 H **ATOM** 663 N VALA 48147.460 9.485 -6.673 1.00 0.00 N 664 CA VALA 48147.149 9.192 -5.280 1.00 0.00 C ATOM 665 C VALA 48147.473 7.740 -4.951 1.00 0.00 C ATOM 666 O VALA 48146.697 6.836 -5.256 1.00 0.00 O ATOM 667 CB VAL A 48145.667 9.463 -4.963 1.00 0.00 C ATOM 668 CG1 VAL A 48145.413 9.366 -3.467 1.00 0.00 C ATOM 669 CG2 VAL A 48145.247 10.826 -5.495 1.00 0.00 C ATOM 670 H VALA 48146.733 9.719 -7.288 1.00 0.00 H ATOM 671 HA VALA 48147.756 9.837 -4.660 1.00 0.00 H **ATOM** 672 HB VALA 48145.070 8.709 -5.456 1.00 0.00 H **ATOM** 673 1HG1 VAL A 48146.110 10.003 -2.942 1.00 0.00 H **ATOM** 674 2HG1 VAL A 48145.547 8.344 -3.145 1.00 0.00 H ATOM 675 3HG1 VAL A 48144.403 9.683 -3.252 1.00 0.00 H **ATOM** 676 1HG2 VAL A 48146.102 11.483 -5.515 1.00 0.00 H ATOM 677 2HG2 VAL A 48144.486 11.244 -4.852 1.00 0.00 H **ATOM** 678 3HG2 VAL A 48144.853 10.716 -6.494 1.00 0.00 H ATOM 679 N LEUA 49148.628 7.523 -4.329 1.00 0.00 N **ATOM** 680 CA LEU A 49149.056 6.179 -3.963 1.00 0.00 C **ATOM** 681 C LEU A 49148.967 5.975 -2.457 1.00 0.00 C **ATOM** 682 O LEUA 49149.649 6.651 -1.687 1.00 0.00 O ATOM 683 CB LEU A 49150.488 5.931 -4.439 1.00 0.00 C ATOM 684 CG LEU A 49150.689 6.006 -5.954 1.00 0.00 C ATOM 685 CD1 LEU A 49152.159 6.205 -6.288 1.00 0.00 C **ATOM** 686 CD2 LEU A 49150.153 4.752 -6.626 1.00 0.00 C **ATOM**

687 H LEU A 49149.206 8.286 -4.112 1.00 0.00 H

ATOM

688 HA LEUA 49148.397 5.477 -4.449 1.00 0.00 H ATOM 689 1HB LEU A 49151.133 6.662 -3.974 1.00 0.00 H ATOM 690 2HB LEU A 49150.789 4.948 -4.109 1.00 0.00 H **ATOM** 691 HG LEUA 49150.142 6.855 -6.341 1.00 0.00 H **ATOM** 692 1HD1 LEU A 49152.669 5.254 -6.248 1.00 0.00 H **ATOM ATOM** 693 2HD1 LEU A 49152.603 6.881 -5.572 1.00 0.00 H 694 3HD1 LEU A 49152.250 6.621 -7.280 1.00 0.00 H **ATOM** 695 1HD2 LEU A 49149.135 4.922 -6.945 1.00 0.00 H ATOM 696 2HD2 LEU A 49150.178 3.930 -5.926 1.00 0.00 H **ATOM** 697 3HD2 LEU A 49150.763 4.513 -7.483 1.00 0.00 H ATOM **ATOM** 698 N ALAA 50148.121 5.041 -2.041 1.00 0.00 N 699 CA ALAA 50147.945 4.752 -0.626 1.00 0.00 C **ATOM** 700 C ALAA 50148.882 3.638 -0.173 1.00 0.00 C **ATOM** 701 O ALAA 50148.766 2.496 -0.616 1.00 0.00 O **ATOM** 702 CB ALAA 50146.498 4.377 -0.339 1.00 0.00 C **ATOM ATOM** 703 H ALAA 50147.603 4.535 -2.702 1.00 0.00 H 704 HA ALAA 50148.175 5.652 -0.075 1.00 0.00 H **ATOM** 705 1HB ALA A 50146.198 4.799 0.610 1.00 0.00 H **ATOM** 706 2HB ALA A 50146.406 3.303 -0.300 1.00 0.00 H **ATOM** 707 3HB ALAA 50145.864 4.766 -1.122 1.00 0.00 H **ATOM** 708 N GLYA 51149.813 3.979 0.712 1.00 0.00 N **ATOM ATOM** 709 CA GLY A 51150.760 2.998 1.211 1.00 0.00 C 710 C GLYA 51150.106 1.965 2.109 1.00 0.00 C ATOM 711 O GLY A 51149.797 2.248 3.266 1.00 0.00 O **ATOM** 712 H GLY A 51149.860 4.905 1.030 1.00 0.00 H **ATOM** 713 1HA GLY A 51151.212 2.492 0.370 1.00 0.00 H **ATOM** 714 2HA GLY A 51151.530 3.507 1.769 1.00 0.00 H **ATOM** 715 N LEUA 52149.894 0.768 1.575 1.00 0.00 N ATOM 716 CA LEU A 52149.273 -0.310 2.338 1.00 0.00 C **ATOM** 717 C LEUA 52150.326 -1.142 3.061 1.00 0.00 C **ATOM** 718 O LEUA 52151.468 -1.243 2.613 1.00 0.00 O **ATOM**

ATOM 719 CB LEU A 52148.444 -1.205 1.414 1.00 0.00 C 720 CG LEUA 52147.167 -0.566 0.868 1.00 0.00 C **ATOM** 721 CD1 LEU A 52146.575 -1.421 -0.242 1.00 0.00 C **ATOM** 722 CD2 LEU A 52146.154 -0.361 1.984 1.00 0.00 C **ATOM** 723 H LEUA 52150.162 0.603 0.647 1.00 0.00 H **ATOM ATOM** 724 HA LEU A 52148.619 0.139 3.071 1.00 0.00 H 725 1HB LEU A 52149.064 -1.496 0.579 1.00 0.00 H ATOM 726 2HB LEU A 52148.168 -2.094 1.963 1.00 0.00 H **ATOM** 727 HG LEUA 52147.407 0.402 0.450 1.00 0.00 H **ATOM** 728 1HD1 LEU A 52146.553 -2.454 0.074 1.00 0.00 H **ATOM** 729 2HD1 LEU A 52147.181 -1.330 -1.131 1.00 0.00 H **ATOM** 730 3HD1 LEU A 52145.569 -1.089 -0.455 1.00 0.00 H **ATOM** 731 1HD2 LEU A 52145.155 -0.488 1.591 1.00 0.00 H **ATOM** 732 2HD2 LEU A 52146.258 0.636 2.386 1.00 0.00 H **ATOM** 733 3HD2 LEU A 52146.329 -1.085 2.765 1.00 0.00 H **ATOM** 734 N GLUA 53149.934 -1.737 4.184 1.00 0.00 N **ATOM** 735 CA GLU A 53150.845 -2.562 4.970 1.00 0.00 C ATOM 736 C GLUA 53150.352 -4.005 5.036 1.00 0.00 C ATOM **ATOM** 737 O GLU A 53149.404 -4.315 5.758 1.00 0.00 O 738 CB GLU A 53150.988 -1.995 6.383 1.00 0.00 C **ATOM** 739 CG GLU A 53151.949 -2.780 7.260 1.00 0.00 C **ATOM** 740 CD GLUA 53151.396 -3.037 8.648 1.00 0.00 C **ATOM** 741 OE1 GLU A 53150.544 -2.245 9.104 1.00 0.00 O **ATOM** 742 OE2 GLU A 53151.814 -4.030 9.281 1.00 0.00 O ATOM 743 H GLUA 53149.011 -1.619 4.490 1.00 0.00 H **ATOM** 744 HA GLU A 53151.809 -2.545 4.486 1.00 0.00 H ATOM 745 1HB GLU A 53151.345 -0.977 6.317 1.00 0.00 H **ATOM** 746 2HB GLU A 53150.018 -1.995 6.859 1.00 0.00 H ATOM 747 1HG GLUA 53152.150 -3.732 6.789 1.00 0.00 H ATOM **ATOM** 748 2HG GLU A 53152.870 -2.223 7.353 1.00 0.00 H 749 N LEUA 54151.002 -4.881 4.279 1.00 0.00 N ATOM

750 CA LEU A 54150.631 -6.290 4.251 1.00 0.00 C ATOM 751 C LEUA 54150.942 -6.961 5.585 1.00 0.00 C **ATOM** 752 O LEUA 54152.009 -6.752 6.162 1.00 0.00 O ATOM 753 CB LEU A 54151.366 -7.013 3.120 1.00 0.00 C 754 CG LEU A 54151.264 -6.341 1.750 1.00 0.00 C **ATOM** 755 CD1 LEU A 54152.286 -6.930 0.790 1.00 0.00 C ATOM 756 CD2 LEU A 54149.857 -6.487 1.190 1.00 0.00 C **ATOM** 757 H LEUA 54151.750 -4.573 3.725 1.00 0.00 H **ATOM ATOM** 758 HA LEU A 54149.568 -6.349 4.072 1.00 0.00 H 759 1HB LEUA 54152.412 -7.083 3.386 1.00 0.00 H **ATOM** 760 2HB LEU A 54150.965 -8.011 3.037 1.00 0.00 H **ATOM** 761 HG LEU A 54151.475 -5.287 1.856 1.00 0.00 H **ATOM** 762 1HD1 LEU A 54153.278 -6.623 1.087 1.00 0.00 H ATOM 763 2HD1 LEU A 54152.086 -6.576 -0.211 1.00 0.00 H **ATOM** 764 3HD1 LEU A 54152.221 -8.007 0.810 1.00 0.00 H **ATOM** 765 1HD2 LEU A 54149.404 -7.383 1.586 1.00 0.00 H ATOM 766 2HD2 LEU A 54149.904 -6.554 0.112 1.00 0.00 H **ATOM** 767 3HD2 LEU A 54149.266 -5.628 1.472 1.00 0.00 H ATOM 768 N GLUA 55150.004 -7.769 6.069 1.00 0.00 N ATOM 769 CA GLU A 55150.179 -8.471 7.335 1.00 0.00 C **ATOM** 770 C GLUA 55151.238 -9.562 7.211 1.00 0.00 C ATOM 771 O GLUA 55151.998 -9.812 8.146 1.00 0.00 O **ATOM** 772 CB GLU A 55148.852 -9.081 7.792 1.00 0.00 C **ATOM** 773 CG GLU A 55147.840 -8.051 8.264 1.00 0.00 C **ATOM** 774 CD GLU A 55146.466 -8.647 8.494 1.00 0.00 C **ATOM** 775 OE1 GLU A 55146.189 -9.080 9.633 1.00 0.00 O **ATOM** 776 OE2 GLU A 55145.665 -8.681 7.536 1.00 0.00 O ATOM 777 H GLUA 55149.175 -7.896 5.562 1.00 0.00 H **ATOM** 778 HA GLUA 55150.505 -7.751 8.071 1.00 0.00 H ATOM 779 1HB GLU A 55148.419 -9.629 6.968 1.00 0.00 H **ATOM** 780 2HB GLU A 55149.045 -9.764 8.605 1.00 0.00 H ATOM

ATOM 781 1HG GLU A 55148.188 -7.621 9.191 1.00 0.00 H 782 2HG GLU A 55147.759 -7.275 7.516 1.00 0.00 H ATOM **ATOM** 783 N ASPA 56151.281 -10.208 6.050 1.00 0.00 N ATOM 784 CA ASP A 56152.247 -11.271 5.804 1.00 0.00 C 785 C ASPA 56153.564 -10.701 5.286 1.00 0.00 C **ATOM** 786 O ASPA 56153.588 -9.960 4.303 1.00 0.00 O ATOM 787 CB ASP A 56151.682 -12.279 4.800 1.00 0.00 C ATOM **ATOM** 788 CG ASP A 56151.146 -13.527 5.473 1.00 0.00 C **ATOM** 789 OD1 ASP A 56151.658 -14.628 5.177 1.00 0.00 O 790 OD2 ASP A 56150.215 -13.404 6.297 1.00 0.00 O **ATOM** 791 H ASPA 56150.649 -9.963 5.342 1.00 0.00 H ATOM 792 HA ASP A 56152.431 -11.775 6.741 1.00 0.00 H **ATOM** 793 1HB ASP A 56150.877 -11.816 4.249 1.00 0.00 H ATOM **ATOM** 794 2HB ASP A 56152.463 -12.571 4.112 1.00 0.00 H **ATOM** 795 N GLUA 57154.658 -11.051 5.955 1.00 0.00 N **ATOM** 796 CA GLU A 57155.979 -10.573 5.561 1.00 0.00 C ATOM 797 C GLUA 57156.430 -11.230 4.261 1.00 0.00 C 798 O GLUA 57157.105 -12.259 4.276 1.00 0.00 O ATOM 799 CB GLU A 57156.996 -10.855 6.669 1.00 0.00 C **ATOM ATOM** 800 CG GLU A 57156.796 -10.001 7.910 1.00 0.00 C **ATOM** 801 CD GLU A 57156.996 -10.782 9.194 1.00 0.00 C 802 OE1 GLU A 57157.428 -10.176 10.197 1.00 0.00 O ATOM **ATOM** 803 OE2 GLU A 57156.719 -12.000 9.197 1.00 0.00 O 804 H GLUA 57154.576 -11.644 6.730 1.00 0.00 H ATOM 805 HA GLU A 57155.913 -9.507 5.409 1.00 0.00 H **ATOM** 806 1HB GLU A 57156.919 -11.893 6.957 1.00 0.00 H ATOM 807 2HB GLU A 57157.988 -10.669 6.287 1.00 0.00 H ATOM 808 1HG GLU A 57157.505 -9.187 7.890 1.00 0.00 H ATOM 809 2HG GLU A 57155.792 -9.603 7.900 1.00 0.00 H ATOM 810 N CYS A 58156.053 -10.627 3.138 1.00 0.00 N ATOM ATOM 811 CA CYS A 58156.420 -11.154 1.829 1.00 0.00 C

- 812 C CYS A 58157.732 -10.544 1.345 1.00 0.00 C 813 O CYS A 58157.972 -9.349 1.513 1.00 0.00 O ATOM 814 CB CYS A 58155.309 -10.874 0.814 1.00 0.00 C 815 SG CYS A 58153.948 -12.062 0.864 1.00 0.00 S **ATOM** 816 H CYS A 58155.515 -9.810 3.192 1.00 0.00 H **ATOM** 817 HA CYS A 58156.546 -12.221 1.924 1.00 0.00 H **ATOM** 818 1HB CYS A 58154.897 -9.894 1.005 1.00 0.00 H **ATOM** 819 2HB CYS A 58155.729 -10.894 -0.181 1.00 0.00 H **ATOM** 820 HG CYS A 58154.203 -12.781 1.445 1.00 0.00 H **ATOM** 821 N ALAA 59158.577 -11.375 0.745 1.00 0.00 N **ATOM** 822 CA ALAA 59159.865 -10.917 0.236 1.00 0.00 C **ATOM** 823 C ALAA 59159.687 -10.014 -0.978 1.00 0.00 C **ATOM** 824 O ALAA 59158.952 -10.344 -1.908 1.00 0.00 O **ATOM** 825 CB ALAA 59160.746 -12.107 -0.115 1.00 0.00 C **ATOM** 826 H ALAA 59158.330 -12.317 0.640 1.00 0.00 H **ATOM** 827 HA ALA A 59160.353 -10.358 1.021 1.00 0.00 H ATOM **ATOM** 828 1HB ALA A 59161.002 -12.643 0.787 1.00 0.00 H 829 2HB ALA A 59161.648 -11.758 -0.595 1.00 0.00 H **ATOM** 830 3HB ALA A 59160.213 -12.765 -0.786 1.00 0.00 H **ATOM** 831 N GLY A 60160.363 -8.869 -0.962 1.00 0.00 N ATOM 832 CA GLY A 60160.266 -7.934 -2.068 1.00 0.00 C **ATOM** 833 C GLY A 60159.640 -6.615 -1.658 1.00 0.00 C **ATOM** 834 O GLY A 60159.930 -5.573 -2.248 1.00 0.00 O **ATOM**
- ATOM 838 N CYS A 61158.781 -6.658 -0.646 1.00 0.00 N

ATOM

ATOM

ATOM

835 H GLY A 60160.933 -8.658 -0.194 1.00 0.00 H

836 1HA GLY A 60161.257 -7.746 -2.453 1.00 0.00 H

837 2HA GLY A 60159.665 -8.377 -2.849 1.00 0.00 H

- ATOM 839 CA CYS A 61158.113 -5.458 -0.159 1.00 0.00 C
- ATOM 840 C CYS A 61159.094 -4.548 0.573 1.00 0.00 C
- ATOM 841 O CYS A 61160.188 -4.971 0.946 1.00 0.00 O
- ATOM 842 CB CYS A 61156.957 -5.833 0.770 1.00 0.00 C

- ATOM 843 SG CYS A 61155.776 -6.994 0.047 1.00 0.00 S
- ATOM 844 H CYS A 61158.591 -7.518 -0.217 1.00 0.00 H
- ATOM 845 HA CYS A 61157.718 -4.928 -1.013 1.00 0.00 H
- ATOM 846 1HB CYS A 61157.357 -6.289 1.665 1.00 0.00 H
- ATOM 847 2HB CYS A 61156.416 -4.937 1.040 1.00 0.00 H
- ATOM 848 HG CYS A 61156.044 -7.882 0.292 1.00 0.00 H
- ATOM 849 N THR A 62158.695 -3.297 0.777 1.00 0.00 N
- ATOM 850 CA THR A 62159.539 -2.327 1.465 1.00 0.00 C
- ATOM 851 C THR A 62159.139 -2.201 2.932 1.00 0.00 C
- ATOM 852 O THR A 62158.254 -2.912 3.407 1.00 0.00 O
- ATOM 853 CB THR A 62159.447 -0.963 0.780 1.00 0.00 C
- ATOM 854 OG1 THR A 62158.176 -0.787 0.179 1.00 0.00 O
- ATOM 855 CG2 THR A 62160.493 -0.761 -0.297 1.00 0.00 C
- ATOM 856 H THR A 62157.811 -3.019 0.456 1.00 0.00 H
- ATOM 857 HA THR A 62160.558 -2.679 1.411 1.00 0.00 H
- ATOM 858 HB THR A 62159.582 -0.189 1.521 1.00 0.00 H
- ATOM 859 HG1 THR A 62157.510 -0.686 0.864 1.00 0.00 H
- ATOM 860 1HG2 THR A 62160.029 -0.340 -1.175 1.00 0.00 H
- ATOM 861 2HG2 THR A 62160.940 -1.712 -0.546 1.00 0.00 H
- ATOM 862 3HG2 THR A 62161.257 -0.089 0.066 1.00 0.00 H
- ATOM 863 N ASPA 63159.797 -1.291 3.642 1.00 0.00 N
- ATOM. 864 CA ASPA 63159.510 -1.071 5.055 1.00 0.00 C
- ATOM 865 C ASP A 63158.823 0.274 5.267 1.00 0.00 C
- ATOM 866 O ASPA 63158.994 0.913 6.306 1.00 0.00 O
- ATOM 867 CB ASPA 63160.800 -1.132 5.874 1.00 0.00 C
- ATOM 868 CG ASP A 63161.816 -0.098 5.431 1.00 0.00 C
- ATOM 869 OD1 ASP A 63162.969 -0.483 5.143 1.00 0.00 O
- ATOM 870 OD2 ASP A 63161.459 1.098 5.371 1.00 0.00 O
- ATOM 871 H ASPA 63160.492 -0.755 3.207 1.00 0.00 H
- ATOM 872 HA ASP A 63158.847 -1.857 5.385 1.00 0.00 H
- ATOM 873 1HB ASP A 63160.568 -0.958 6.914 1.00 0.00 H

874 2HB ASPA 63161.241 -2.113 5.768 1.00 0.00 H 875 N GLY A 64158.045 0.698 4.277 1.00 0.00 N **ATOM** 876 CA GLY A 64157.344 1.966 4.375 1.00 0.00 C **ATOM** 877 C GLY A 64158.028 3.069 3.593 1.00 0.00 C **ATOM** 878 O GLY A 64158.120 4.204 4.059 1.00 0.00 O **ATOM** 879 H GLY A 64157.946 0.148 3.473 1.00 0.00 H ATOM **ATOM** 880 1HA GLY A 64156.341 1.839 3.997 1.00 0.00 H 881 2HA GLY A 64157.292 2.255 5.414 1.00 0.00 H **ATOM** 882 N THR A 65158.508 2.736 2.400 1.00 0.00 N **ATOM** 883 CA THR A 65159.188 3.707 1.550 1.00 0.00 C **ATOM** 884 C THR A 65158.823 3.496 0.083 1.00 0.00 C **ATOM ATOM** 885 O THR A 65158.776 2.365 -0.399 1.00 0.00 O 886 CB THR A 65160.703 3.602 1.730 1.00 0.00 C **ATOM** 887 OG1 THR A 65161.154 2.295 1.424 1.00 0.00 O **ATOM** 888 CG2 THR A 65161.162 3.928 3.135 1.00 0.00 C **ATOM** 889 H THR A 65158.403 1.814 2.083 1.00 0.00 H ATOM 890 HA THR A 65158.865 4.692 1.850 1.00 0.00 H ATOM 891 HB THR A 65161.184 4.295 1.056 1.00 0.00 H ATOM 892 HG1 THR A 65160.864 2.054 0.541 1.00 0.00 H ATOM 893 1HG2 THR A 65160.333 4.326 3.701 1.00 0.00 H ATOM 894 2HG2 THR A 65161.954 4.661 3.094 1.00 0.00 H **ATOM** 895 3HG2 THR A 65161.526 3.031 3.613 1.00 0.00 H **ATOM** 896 N PHE A 66158.565 4.594 -0.621 1.00 0.00 N **ATOM** 897 CA PHE A 66158.205 4.530 -2.032 1.00 0.00 C **ATOM** 898 C PHE A 66159.340 5.050 -2.907 1.00 0.00 C ATOM 899 O PHE A 66159.609 6.250 -2.942 1.00 0.00 O **ATOM** 900 CB PHE A 66156.933 5.338 -2.293 1.00 0.00 C **ATOM** 901 CG PHE A 66156.226 4.951 -3.560 1.00 0.00 C **ATOM** 902 CD1 PHE A 66155.795 3.648 -3.758 1.00 0.00 C ATOM 903 CD2 PHE A 66155.992 5.888 -4.553 1.00 0.00 C **ATOM** ATOM 904 CE1 PHE A 66155.145 3.289 -4.923 1.00 0.00 C

ATOM 905 CE2 PHE A 66155.343 5.534 -5.721 1.00 0.00 C 906 CZ PHE A 66154.919 4.232 -5.906 1.00 0.00 C **ATOM** 907 H PHE A 66158.618 5.468 -0.181 1.00 0.00 H **ATOM** ATOM 908 HA PHE A 66158.020 3.494 -2.280 1.00 0.00 H **ATOM** 909 1HB PHE A 66156.247 5.191 -1.472 1.00 0.00 H ATOM 910 2HB PHE A 66157.188 6.385 -2.360 1.00 0.00 H 911 HD1 PHE A 66155.971 2.909 -2.990 1.00 0.00 H **ATOM** 912 HD2 PHE A 66156.324 6.906 -4.409 1.00 0.00 H **ATOM** 913 HE1 PHE A 66154.815 2.270 -5.065 1.00 0.00 H ATOM 914 HE2 PHE A 66155.167 6.273 -6.487 1.00 0.00 H ATOM 915 HZ PHE A 66154.411 3.953 -6.818 1.00 0.00 H ATOM 916 N ARGA 67160.001 4.139 -3.614 1.00 0.00 N ATOM ATOM 917 CA ARG A 67161.107 4.506 -4.490 1.00 0.00 C 918 C ARGA 67162.211 5.212 -3.708 1.00 0.00 C **ATOM** 919 O ARGA 67162.933 6.048 -4.251 1.00 0.00 O **ATOM ATOM** 920 CB ARG A 67160.612 5.408 -5.622 1.00 0.00 C 921 CG ARG A 67159.489 4.794 -6.441 1.00 0.00 C ATOM ATOM 922 CD ARG A 67158.923 5.788 -7.443 1.00 0.00 C **ATOM** 923 NE ARG A 67157.777 5.245 -8.167 1.00 0.00 N 924 CZ ARG A 67157.880 4.402 -9.192 1.00 0.00 C **ATOM** 925 NH1 ARG A 67159.073 4.005 -9.618 1.00 0.00 N **ATOM ATOM** 926 NH2 ARG A 67156.787 3.955 -9.795 1.00 0.00 N 927 H ARG A 67159.739 3.197 -3.544 1.00 0.00 H ATOM **ATOM** 928 HA ARG A 67161.509 3.598 -4.915 1.00 0.00 H 929 1HB ARG A 67160.253 6.334 -5.197 1.00 0.00 H ATOM 930 2HB ARG A 67161.437 5.622 -6.285 1.00 0.00 H **ATOM ATOM** 931 1HG ARG A 67159.873 3.939 -6.977 1.00 0.00 H 932 2HG ARG A 67158.699 4.480 -5.775 1.00 0.00 H ATOM ATOM 933 1HD ARG A 67158.613 6.677 -6.912 1.00 0.00 H 934 2HD ARG A 67159.697 6.046 -8.152 1.00 0.00 H ATOM ATOM 935 HE ARG A 67156.884 5.521 -7.874 1.00 0.00 H

936 1HH1 ARG A 67159.902 4.339 -9.169 1.00 0.00 H **ATOM** 937 2HH1 ARG A 67159.143 3.372 -10.389 1.00 0.00 H ATOM ATOM 938 1HH2 ARG A 67155.885 4.251 -9.479 1.00 0.00 H 939 2HH2 ARG A 67156.864 3.323 -10.566 1.00 0.00 H ATOM **ATOM** 940 N GLY A 68162.335 4.871 -2.429 1.00 0.00 N 941 CA GLY A 68163.353 5.483 -1.595 1.00 0.00 C ATOM 942 C GLYA 68162.794 6.570 -0.696 1.00 0.00 C **ATOM** 943 O GLY A 68163.408 6.925 0.310 1.00 0.00 O ATOM 944 H GLY A 68161.732 4.199 -2.049 1.00 0.00 H **ATOM** ATOM 945 1HA GLY A 68163.803 4.719 -0.979 1.00 0.00 H 946 2HA GLY A 68164.112 5.912 -2.231 1.00 0.00 H **ATOM** 947 N THR A 69161.630 7.102 -1.058 1.00 0.00 N **ATOM** 948 CA THR A 69160.995 8.154 -0.275 1.00 0.00 C **ATOM** 949 C THR A 69160.179 7.565 0.871 1.00 0.00 C ATOM 950 O THR A 69159.128 6.961 0.651 1.00 0.00 O ATOM 951 CB THR A 69160.098 9.013 -1.167 1.00 0.00 C **ATOM** 952 OG1 THR A 69160.773 9.370 -2.361 1.00 0.00 O ATOM 953 CG2 THR A 69159.637 10.290 -0.501 1.00 0.00 C **ATOM** 954 H THR A 69161.188 6.779 -1.870 1.00 0.00 H ATOM 955 HA THR A 69161.776 8.776 0.139 1.00 0.00 H ATOM 956 HB THR A 69159.220 8.442 -1.432 1.00 0.00 H ATOM 957 HG1 THR A 69161.532 9.917 -2.148 1.00 0.00 H ATOM 958 1HG2 THR A 69159.314 10.994 -1.255 1.00 0.00 H ATOM 959 2HG2 THR A 69160.453 10.717 0.064 1.00 0.00 H **ATOM** 960 3HG2 THR A 69158.814 10.073 0.164 1.00 0.00 H **ATOM** 961 N ARG A 70160.668 7.743 2.093 1.00 0.00 N **ATOM** 962 CA ARG A 70159.984 7.230 3.273 1.00 0.00 C ATOM 963 C ARG A 70158.798 8.116 3.643 1.00 0.00 C ATOM

471

964 O ARG A 70158.936 9.332 3.770 1.00 0.00 O

965 CB ARG A 70160.953 7.139 4.452 1.00 0.00 C

966 CG ARG A 70160.326 6.570 5.714 1.00 0.00 C

ATOM

ATOM

ATOM

ATOM 967 CD ARG A 70160.985 7.127 6.965 1.00 0.00 C 968 NE ARG A 70162.129 6.321 7.387 1.00 0.00 N **ATOM** ATOM 969 CZ ARG A 70162.855 6.575 8.472 1.00 0.00 C ATOM 970 NH1 ARG A 70162.559 7.610 9.250 1.00 0.00 N 971 NH2 ARG A 70163.880 5.793 8.782 1.00 0.00 N ATOM ATOM 972 H ARG A 70161.509 8.234 2.205 1.00 0.00 H 973 HA ARG A 70159.619 6.241 3.041 1.00 0.00 H **ATOM** ATOM 974 1HB ARG A 70161.783 6.507 4.174 1.00 0.00 H 975 2HB ARG A 70161.325 8.128 4.676 1.00 0.00 H **ATOM** 976 1HG ARG A 70159.277 6.825 5.730 1.00 0.00 H ATOM 977 2HG ARG A 70160.437 5.495 5.708 1.00 0.00 H **ATOM ATOM** 978 1HD ARG A 70161.321 8.133 6.762 1.00 0.00 H ATOM 979 2HD ARG A 70160.257 7.147 7.763 1.00 0.00 H **ATOM** 980 HE ARG A 70162.369 5.551 6.830 1.00 0.00 H 981 1HH1 ARG A 70161.788 8.203 9.022 1.00 0.00 H **ATOM** ATOM 982 2HH1 ARG A 70163.108 7.795 10.066 1.00 0.00 H 983 1HH2 ARG A 70164.106 5.012 8.201 1.00 0.00 H ATOM ATOM 984 2HH2 ARG A 70164.426 5.984 9.599 1.00 0.00 H 985 N TYR A 71157.633 7.498 3.811 1.00 0.00 N ATOM 986 CA TYR A 71156.424 8.231 4.165 1.00 0.00 C **ATOM** 987 C TYR A 71155.976 7.891 5.583 1.00 0.00 C ATOM 988 O TYR A 71155.657 8.779 6.373 1.00 0.00 O **ATOM** 989 CB TYR A 71155.302 7.914 3.175 1.00 0.00 C ATOM **ATOM** 990 CG TYR A 71155.508 8.530 1.808 1.00 0.00 C 991 CD1 TYR A 71155.560 9.908 1.648 1.00 0.00 C **ATOM** 992 CD2 TYR A 71155.651 7.731 0.681 1.00 0.00 C **ATOM** 993 CE1 TYR A 71155.748 10.475 0.401 1.00 0.00 C ATOM 994 CE2 TYR A 71155.840 8.290 -0.569 1.00 0.00 C ATOM ATOM 995 CZ TYR A 71155.888 9.661 -0.703 1.00 0.00 C ATOM 996 OH TYR A 71156.075 10.221 -1.946 1.00 0.00 O ATOM 997 H TYR A 71157.587 6.526 3.695 1.00 0.00 H

ATOM 998 HA TYR A 71156.648 9.286 4.115 1.00 0.00 H ATOM 999 1HB TYR A 71155.234 6.844 3.048 1.00 0.00 H ATOM 1000 2HB TYR A 71154.368 8.285 3.569 1.00 0.00 H ATOM 1001 HD1 TYR A 71155.450 10.542 2.515 1.00 0.00 H ATOM 1002 HD2 TYR A 71155.613 6.657 0.788 1.00 0.00 H ATOM 1003 HE1 TYR A 71155.785 11.549 0.297 1.00 0.00 H ATOM 1004 HE2 TYR A 71155.950 7.654 -1.435 1.00 0.00 H ATOM 1005 HH TYR A 71155.283 10.101 -2.476 1.00 0.00 H ATOM 1006 N PHE A 72155.956 6.600 5.898 1.00 0.00 N ATOM 1007 CA PHE A 72155.548 6.144 7.222 1.00 0.00 C ATOM 1008 C PHE A 72156.530 5.113 7.768 1.00 0.00 C ATOM 1009 O PHE A 72157.388 4.612 7.042 1.00 0.00 O ATOM 1010 CB PHE A 72154.141 5.546 7.167 1.00 0.00 C ATOM 1011 CG PHE A 72153,971 4,509 6.093 1.00 0.00 C ATOM 1012 CD1 PHE A 72153.819 4.884 4.768 1.00 0.00 C ATOM 1013 CD2 PHE A 72153.963 3.161 6.410 1.00 0.00 C ATOM 1014 CE1 PHE A 72153.663 3.932 3.779 1.00 0.00 C ATOM 1015 CE2 PHE A 72153.806 2.204 5.425 1.00 0.00 C ATOM 1016 CZ PHE A 72153.657 2.590 4.107 1.00 0.00 C ATOM 1017 H PHE A 72156.222 5.940 5.226 1.00 0.00 H ATOM 1018 HA PHE A 72155.540 7.000 7.880 1.00 0.00 H ATOM 1019 1HB PHE A 72153.917 5.082 8.115 1.00 0.00 H ATOM 1020 2HB PHE A 72153.428 6.338 6.982 1.00 0.00 H ATOM 1021 HD1 PHE A 72153.824 5.932 4.509 1.00 0.00 H ATOM 1022 HD2 PHE A 72154.080 2.857 7.440 1.00 0.00 H ATOM 1023 HE1 PHE A 72153.545 4.237 2.749 1.00 0.00 H ATOM 1024 HE2 PHE A 72153.803 1.155 5.685 1.00 0.00 H ATOM 1025 HZ PHE A 72153.534 1.844 3.335 1.00 0.00 H ATOM 1026 N THR A 73156.397 4.800 9.053 1.00 0.00 N ATOM 1027 CA THR A 73157.272 3.828 9.698 1.00 0.00 C ATOM 1028 C THR A 73156.519 2.538 10.005 1.00 0.00 C

ATOM 1029 O THR A 73155.738 2.473 10.954 1.00 0.00 O ATOM 1030 CB THR A 73157.854 4.411 10.986 1.00 0.00 C ATOM 1031 OG1 THR A 73158.089 5.800 10.847 1.00 0.00 O ATOM 1032 CG2 THR A 73159.160 3.764 11.400 1.00 0.00 C ATOM 1033 H THR A 73155.693 5.232 9.581 1.00 0.00 H ATOM 1034 HA THR A 73158.080 3.606 9.016 1.00 0.00 H ATOM 1035 HB THR A 73157.145 4.265 11.788 1.00 0.00 H ATOM 1036 HG1 THR A 73158.193 6.197 11.715 1.00 0.00 H ATOM 1037 1HG2 THR A 73159.299 3.884 12.464 1.00 0.00 H ATOM 1038 2HG2 THR A 73159.977 4.235 10.874 1.00 0.00 H ATOM 1039 3HG2 THR A 73159.133 2.712 11.155 1.00 0.00 H ATOM 1040 N CYS A 74156.759 1.511 9.195 1.00 0.00 N ATOM 1041 CA CYS A 74156.104 0.222 9.380 1.00 0.00 C ATOM 1042 C CYS A 74157.120 -0.916 9.346 1.00 0.00 C ATOM 1043 O CYS A 74158.299 -0.699 9.070 1.00 0.00 O ATOM 1044 CB CYS A 74155.043 0.005 8.299 1.00 0.00 C ATOM 1045 SG CYS A 74153.400 0.615 8.745 1.00 0.00 S ATOM 1046 H CYS A 74157.392 1.624 8.455 1.00 0.00 H ATOM 1047 HA CYS A 74155.623 0.231 10.346 1.00 0.00 H ATOM 1048 1HB CYS A 74155.349 0.516 7.398 1.00 0.00 H ATOM 1049 2HB CYS A 74154.958 -1.052 8.095 1.00 0.00 H ATOM 1050 HG CYS A 74153.461 1.565 8.873 1.00 0.00 H ATOM 1051 N ALA A 75156.654 -2.127 9.629 1.00 0.00 N ATOM 1052 CA ALA A 75157.521 -3.299 9.631 1.00 0.00 C ATOM 1053 C ALAA 75158.160 -3.510 8.263 1.00 0.00 C ATOM 1054 O ALAA 75157.646 -3.043 7.247 1.00 0.00 O ATOM 1055 CB ALA A 75156.737 -4.534 10.046 1.00 0.00 C ATOM 1056 H ALA A 75155.703 -2.236 9.841 1.00 0.00 H ATOM 1057 HA ALA A 75158.301 -3.134 10.359 1.00 0.00 H ATOM 1058 1HB ALAA 75157.146 -5.403 9.551 1.00 0.00 H ATOM 1059 2HB ALA A 75155.701 -4.415 9.767 1.00 0.00 H

ATOM 1060 3HB ALAA 75156.810 -4.663 11.116 1.00 0.00 H ATOM 1061 N LEUA 76159.285 -4.219 8.243 1.00 0.00 N ATOM 1062 CA LEU A 76159.994 -4.493 6.999 1.00 0.00 C ATOM 1063 C LEUA 76159.283 -5.576 6.194 1.00 0.00 C ATOM 1064 O LEU A 76158.703 -6.503 6.759 1.00 0.00 O ATOM 1065 CB LEU A 76161.433 -4.921 7.291 1.00 0.00 C ATOM 1066 CG LEU A 76162.351 -3.804 7.794 1.00 0.00 C ATOM 1067 CD1 LEU A 76162.435 -3.826 9.312 1.00 0.00 C ATOM 1068 CD2 LEU A 76163.736 -3.934 7.179 1.00 0.00 C ATOM 1069 H LEU A 76159.645 -4.567 9.085 1.00 0.00 H ATOM 1070 HA LEU A 76160.009 -3.583 6.419 1.00 0.00 H ATOM 1071 1HB LEU A 76161.410 -5.702 8.036 1.00 0.00 H ATOM 1072 2HB LEU A 76161.858 -5.324 6.383 1.00 0.00 H ATOM 1073 HG LEU A 76161.940 -2.849 7.497 1.00 0.00 H ATOM 1074 1HD1 LEU A 76162.427 -4.848 9.658 1.00 0.00 H ATOM 1075 2HD1 LEU A 76161.591 -3.298 9.728 1.00 0.00 H ATOM 1076 3HD1 LEU A 76163.350 -3.346 9.628 1.00 0.00 H ATOM 1077 1HD2 LEU A 76163.645 -4.063 6.111 1.00 0.00 H ATOM 1078 2HD2 LEU A 76164.240 -4.790 7.603 1.00 0.00 H ATOM 1079 3HD2 LEU A 76164.307 -3.041 7.386 1.00 0.00 H ATOM 1080 N LYS A 77159.332 -5.452 4.872 1.00 0.00 N ATOM 1081 CA LYS A 77158.692 -6.421 3.989 1.00 0.00 C ATOM 1082 C LYS A 77157.190 -6.481 4.245 1.00 0.00 C ATOM 1083 O LYS A 77156.565 -7.528 4.083 1.00 0.00 O ATOM 1084 CB LYS A 77159.310 -7.807 4.186 1.00 0.00 C ATOM 1085 CG LYS A 77160.806 -7.849 3.921 1.00 0.00 C ATOM 1086 CD LYS A 77161.117 -7.641 2.448 1.00 0.00 C ATOM 1087 CE LYS A 77162.396 -6.843 2.255 1.00 0.00 C ATOM 1088 NZ LYS A 77163.575 -7.532 2.849 1.00 0.00 N ATOM 1089 H LYS A 77159.809 -4.692 4.480 1.00 0.00 H ATOM 1090 HA LYS A 77158.860 -6.103 2.971 1.00 0.00 H

ATOM 1091 1HB LYS A 77159.138 -8.124 5.203 1.00 0.00 H ATOM 1092 2HB LYS A 77158.828 -8.502 3.515 1.00 0.00 H ATOM 1093 1HG LYS A 77161.285 -7.069 4.493 1.00 0.00 H ATOM 1094 2HG LYS A 77161.190 -8.811 4.228 1.00 0.00 H ATOM 1095 1HD LYS A 77161.231 -8.604 1.973 1.00 0.00 H ATOM 1096 2HD LYS A 77160.298 -7.107 1.989 1.00 0.00 H ATOM 1097 1HE LYS A 77162.566 -6.708 1.197 1.00 0.00 H ATOM 1098 2HE LYS A 77162.279 -5.879 2.726 1.00 0.00 H ATOM 1099 1HZ LYS A 77163.556 -8.544 2.608 1.00 0.00 H ATOM 1100 2HZ LYS A 77163.563 -7.433 3.884 1.00 0.00 H ATOM 1101 3HZ LYS A 77164.455 -7.116 2.482 1.00 0.00 H ATOM 1102 N LYS A 78156.617 -5.350 4.644 1.00 0.00 N ATOM 1103 CA LYS A 78155.188 -5.274 4.922 1.00 0.00 C ATOM 1104 C LYS A 78154.619 -3.926 4.490 1.00 0.00 C ATOM 1105 O LYS A 78153.788 -3.339 5.184 1.00 0.00 O ATOM 1106 CB LYS A 78154.924 -5.500 6.412 1.00 0.00 C ATOM 1107 CG LYS A 78155.426 -6.841 6.922 1.00 0.00 C ATOM 1108 CD LYS A 78155.126 -7.022 8.401 1.00 0.00 C ATOM 1109 CE LYS A 78153.865 -7.842 8.618 1.00 0.00 C ATOM 1110 NZ LYS A 78153.075 -7.350 9.780 1.00 0.00 N ATOM 1111 H LYS A 78157.169 -4.548 4.754 1.00 0.00 H ATOM 1112 HA LYS A 78154.699 -6.054 4.357 1.00 0.00 H ATOM 1113 1HB LYS A 78155.414 -4.719 6.974 1.00 0.00 H ATOM 1114 2HB LYS A 78153.860 -5.447 6.589 1.00 0.00 H ATOM 1115 1HG LYS A 78154.941 -7.631 6.368 1.00 0.00 H ATOM 1116 2HG LYS A 78156.494 -6.896 6.771 1.00 0.00 H ATOM 1117 1HD LYS A 78155.958 -7.528 8.868 1.00 0.00 H ATOM 1118 2HD LYS A 78154.995 -6.049 8.853 1.00 0.00 H ATOM 1119 1HE LYS A 78153.256 -7.784 7.728 1.00 0.00 H ATOM 1120 2HE LYS A 78154.146 -8.870 8.794 1.00 0.00 H ATOM 1121 1HZ LYS A 78153.198 -6.322 9.886 1.00 0.00 H

ATOM 1122 2HZ LYS A 78153.391 -7.818 10.652 1.00 0.00 H ATOM 1123 3HZ LYS A 78152.065 -7.553 9.636 1.00 0.00 H ATOM 1124 N ALA A 79155.073 -3.438 3.340 1.00 0.00 N ATOM 1125 CA ALA A 79154.611 -2.159 2.815 1.00 0.00 C ATOM 1126 C ALA A 79154.473 -2.206 1.297 1.00 0.00 C ATOM 1127 O ALA A 79155.469 -2.255 0.575 1.00 0.00 O ATOM 1128 CB ALA A 79155.562 -1.046 3.227 1.00 0.00 C ATOM 1129 H ALAA 79155.735 -3.953 2.831 1.00 0.00 H ATOM 1130 HA ALA A 79153.643 -1.953 3.249 1.00 0.00 H ATOM 1131 1HB ALA A 79156.567 -1.436 3.292 1.00 0.00 H ATOM 1132 2HB ALA A 79155.265 -0.656 4.190 1.00 0.00 H ATOM 1133 3HB ALA A 79155.529 -0.255 2.494 1.00 0.00 H ATOM 1134 N LEUA 80153.233 -2.190 0.821 1.00 0.00 N ATOM 1135 CA LEU A 80152.964 -2.230 -0.613 1.00 0.00 C ATOM 1136 C LEUA 80152.171 -1.005 -1.052 1.00 0.00 C ATOM 1137 O LEUA 80151.011 -0.836 -0.677 1.00 0.00 O ATOM 1138 CB LEU A 80152.198 -3.505 -0.972 1.00 0.00 C ATOM 1139 CG LEU A 80151.803 -3.630 -2.444 1.00 0.00 C ATOM 1140 CD1 LEU A 80152.954 -4.198 -3.260 1.00 0.00 C ATOM 1141 CD2 LEU A 80150.564 -4.499 -2.591 1.00 0.00 C ATOM 1142 H LEUA 80152.480 -2.151 1.447 1.00 0.00 H ATOM 1143 HA LEU A 80153.913 -2.235 -1.128 1.00 0.00 H ATOM 1144 1HB LEU A 80152.812 -4.355 -0.712 1.00 0.00 H ATOM 1145 2HB LEU A 80151.297 -3.538 -0.379 1.00 0.00 H ATOM 1146 HG LEU A 80151.573 -2.648 -2.834 1.00 0.00 H ATOM 1147 1HD1 LEU A 80153.063 -5.251 -3.044 1.00 0.00 H ATOM 1148 2HD1 LEU A 80153.868 -3.683 -3.001 1.00 0.00 H ATOM 1149 3HD1 LEU A 80152.752 -4.064 -4.312 1.00 0.00 H ATOM 1150 1HD2 LEU A 80149.693 -3.939 -2.281 1.00 0.00 H ATOM 1151 2HD2 LEU A 80150.665 -5.378 -1.973 1.00 0.00 H ATOM 1152 3HD2 LEU A 80150.452 -4.796 -3.624 1.00 0.00 H

ATOM 1153 N PHE A 81152.805 -0.150 -1.849 1.00 0.00 N ATOM 1154 CA PHE A 81152.158 1.061 -2.340 1.00 0.00 C ATOM 1155 C PHE A 81151.313 0.763 -3.574 1.00 0.00 C ATOM 1156 O PHE A 81151.726 0.010 -4.455 1.00 0.00 O ATOM 1157 CB PHE A 81153.206 2.125 -2.670 1.00 0.00 C ATOM 1158 CG PHE A 81153.920 2.660 -1.461 1.00 0.00 C ATOM 1159 CD1 PHE A 81153.537 3.860 -0.888 1.00 0.00 C ATOM 1160 CD2 PHE A 81154.977 1.960 -0.900 1.00 0.00 C ATOM 1161 CE1 PHE A 81154.192 4.354 0.224 1.00 0.00 C ATOM 1162 CE2 PHE A 81155.636 2.449 0.211 1.00 0.00 C ATOM 1163 CZ PHE A 81155.243 3.648 0.774 1.00 0.00 C ATOM 1164 H PHE A 81153.730 -0.339 -2.114 1.00 0.00 H ATOM 1165 HA PHE A 81151.514 1.433 -1.557 1.00 0.00 H ATOM 1166 1HB PHE A 81153,945 1,700 -3,332 1.00 0.00 H ATOM 1167 2HB PHE A 81152.722 2.955 -3.165 1.00 0.00 H ATOM 1168 HD1 PHE A 81152.714 4.414 -1.317 1.00 0.00 H ATOM 1169 HD2 PHE A 81155.285 1.023 -1.339 1.00 0.00 H ATOM 1170 HE1 PHE A 81153.883 5.292 0.661 1.00 0.00 H ATOM 1171 HE2 PHE A 81156.457 1.894 0.641 1.00 0.00 H ATOM 1172 HZ PHE A 81155.757 4.032 1.644 1.00 0.00 H ATOM 1173 N VALA 82150.126 1.359 -3.631 1.00 0.00 N ATOM 1174 CA VALA 82149.223 1.158 -4.757 1.00 0.00 C ATOM 1175 C VALA 82148.323 2.371 -4.966 1.00 0.00 C ATOM 1176 O VALA 82148.239 3.249 -4.107 1.00 0.00 O ATOM 1177 CB VALA 82148.343 -0.089 -4.555 1.00 0.00 C ATOM 1178 CG1 VAL A 82149.177 -1.357 -4.665 1.00 0.00 C ATOM 1179 CG2 VAL A 82147.629 -0.028 -3.213 1.00 0.00 C ATOM 1180 H VALA 82149.852 1.950 -2.898 1.00 0.00 H ATOM 1181 HA VALA 82149.823 1.010 -5.643 1.00 0.00 H ATOM 1182 HB VALA 82147.596 -0.109 -5.334 1.00 0.00 H ATOM 1183 1HG1 VAL A 82149.983 -1.321 -3.947 1.00 0.00 H

ATOM 1184 2HG1 VALA 82149.587 -1.432 -5.661 1.00 0.00 H ATOM 1185 3HG1 VAL A 82148.556 -2.216 -4.465 1.00 0.00 H ATOM 1186 1HG2 VAL A 82146.883 -0.806 -3.165 1.00 0.00 H ATOM 1187 2HG2 VAL A 82147.152 0.935 -3.103 1.00 0.00 H ATOM 1188 3HG2 VAL A 82148.346 -0.167 -2.417 1.00 0.00 H ATOM 1189 N LYS A 83147.653 2.413 -6.112 1.00 0.00 N ATOM 1190 CA LYS A 83146.759 3.518 -6.435 1.00 0.00 C ATOM 1191 C LYS A 83145.547 3.527 -5.510 1.00 0.00 C ATOM 1192 O LYS A 83144.812 2.544 -5.422 1.00 0.00 O ATOM 1193 CB LYS A 83146.301 3.423 -7.892 1.00 0.00 C ATOM 1194 CG LYS A 83147.421 3.629 -8.897 1.00 0.00 C ATOM 1195 CD LYS A 83147.023 3.147-10.283 1.00 0.00 C ATOM 1196 CE LYS A 83147.507 4.099 -11.366 1.00 0.00 C ATOM 1197 NZ LYS A 83147.866 3.380 -12.619 1.00 0.00 N ATOM 1198 H LYS A 83147.762 1.683 -6.757 1.00 0.00 H ATOM 1199 HA LYS A 83147.306 4.439 -6.299 1.00 0.00 H ATOM 1200 1HB LYS A 83145.873 2.445 -8.058 1.00 0.00 H ATOM 1201 2HB LYS A 83145.544 4.173 -8.070 1.00 0.00 H ATOM 1202 1HG LYS A 83147.658 4.682 -8.948 1.00 0.00 H ATOM 1203 2HG LYS A 83148.292 3.079 -8.570 1.00 0.00 H ATOM 1204 1HD LYS A 83147.459 2.174 -10.454 1.00 0.00 H ATOM 1205 2HD LYS A 83145.947 3.075 -10.333 1.00 0.00 H ATOM 1206 1HE LYS A 83146.721 4.808 -11.580 1.00 0.00 H ATOM 1207 2HE LYS A 83148.376 4.627 -11.001 1.00 0.00 H ATOM 1208 1HZ LYS A 83147.045 3.341 -13.256 1.00 0.00 H ATOM 1209 2HZ LYS A 83148.167 2.410 -12.400 1.00 0.00 H ATOM 1210 3HZ LYS A 83148.645 3.872 -13.102 1.00 0.00 H ATOM 1211 N LEUA 84145.347 4.646 -4.823 1.00 0.00 N ATOM 1212 CA LEU A 84144.226 4.791 -3.902 1.00 0.00 C ATOM 1213 C LEU A 84142.898 4.603 -4.630 1.00 0.00 C ATOM 1214 O LEUA 84141.947 4.052 -4.074 1.00 0.00 O

ATOM 1215 CB LEU A 84144.268 6.169 -3.238 1.00 0.00 C ATOM 1216 CG LEU A 84143.081 6.486 -2.326 1.00 0.00 C ATOM 1217 CD1 LEU A 84143.224 5.767 -0.994 1.00 0.00 C ATOM 1218 CD2 LEU A 84142.961 7.988 -2.113 1.00 0.00 C ATOM 1219 H LEUA 84145.970 5.394 -4.938 1.00 0.00 H ATOM 1220 HA LEU A 84144.320 4.031 -3.143 1.00 0.00 H ATOM 1221 1HB LEU A 84145.173 6.234 -2.652 1.00 0.00 H ATOM 1222 2HB LEU A 84144.307 6.918 -4.014 1.00 0.00 H ATOM 1223 HG LEU A 84142.172 6.140 -2.796 1.00 0.00 H ATOM 1224 1HD1 LEU A 84142.368 5.985 -0.373 1.00 0.00 H ATOM 1225 2HD1 LEU A 84144.122 6.103 -0.498 1.00 0.00 H ATOM 1226 3HD1 LEU A 84143.283 4.702 -1.164 1.00 0.00 H ATOM 1227 1HD2 LEU A 84142.120 8.193 -1.467 1.00 0.00 H ATOM 1228 2HD2 LEU A 84142.812 8.475 -3.065 1.00 0.00 H ATOM 1229 3HD2 LEU A 84143.866 8.360 -1.656 1.00 0.00 H ATOM 1230 N LYS A 85142.840 5.064 -5.874 1.00 0.00 N ATOM 1231 CA LYS A 85141.630 4.946 -6.678 1.00 0.00 C ATOM 1232 C LYS A 85141.289 3.482 -6.943 1.00 0.00 C ATOM 1233 O LYS A 85140.129 3.137 -7.171 1.00 0.00 O ATOM 1234 CB LYS A 85141.799 5.690 -8.004 1.00 0.00 C ATOM 1235 CG LYS A 85143.086 5.346 -8.735 1.00 0.00 C ATOM 1236 CD LYS A 85143.011 5.729 -10.204 1.00 0.00 C ATOM 1237 CE LYS A 85142.658 4.534 -11.076 1.00 0.00 C ATOM 1238 NZ LYS A 85143.845 4.006 -11.803 1.00 0.00 N ATOM 1239 H LYS A 85143.631 5.494 -6.263 1.00 0.00 H ATOM 1240 HA LYS A 85140.820 5.396 -6.124 1.00 0.00 H ATOM 1241 1HB LYS A 85140.967 5.446 -8.649 1.00 0.00 H ATOM 1242 2HB LYS A 85141.793 6.753 -7.811 1.00 0.00 H ATOM 1243 1HG LYS A 85143.904 5.880 -8.275 1.00 0.00 H ATOM 1244 2HG LYS A 85143.259 4.282 -8.657 1.00 0.00 H ATOM 1245 1HD LYS A 85142.255 6.489 -10.331 1.00 0.00 H ATOM 1246 2HD LYS A 85143.971 6.117 -10.514 1.00 0.00 H ATOM 1247 1HE LYS A 85142.255 3.752 -10.448 1.00 0.00 H ATOM 1248 2HE LYS A 85141.911 4.837 -11.794 1.00 0.00 H ATOM 1249 1HZ LYS A 85143.815 2.966 -11.830 1.00 0.00 H ATOM 1250 2HZ LYS A 85144.720 4.302 -11.326 1.00 0.00 H ATOM 1251 3HZ LYS A 85143.857 4.367 -12.779 1.00 0.00 H ATOM 1252 N SER A 86142.305 2.625 -6.914 1.00 0.00 N ATOM 1253 CA SER A 86142.110 1.200 -7.152 1.00 0.00 C ATOM 1254 C SER A 86142.025 0.432 -5:835 1.00 0.00 C ATOM 1255 O SER A 86142.396 -0.739 -5.764 1.00 0.00 O ATOM 1256 CB SER A 86143.248 0.644 -8.007 1.00 0.00 C ATOM 1257 OG SER A 86143.129 1.068 -9.354 1.00 0.00 O ATOM 1258 H SER A 86143.208 2.958 -6.728 1.00 0.00 H ATOM 1259 HA SER A 86141.179 1.078 -7.685 1.00 0.00 H ATOM 1260 1HB SER A 86144.193 0.991 -7.616 1.00 0.00 H ATOM 1261 2HB SER A 86143.223 -0.437 -7.979 1.00 0.00 H ATOM 1262 HG SER A 86142.218 0.969 -9.642 1.00 0.00 H ATOM 1263 N CYS A 87141.536 1.101 -4.796 1.00 0.00 N ATOM 1264 CA CYS A 87141.402 0.481 -3.483 1.00 0.00 C ATOM 1265 C CYS A 87139.936 0.392 -3.070 1.00 0.00 C ATOM 1266 O CYS A 87139.121 1.231 -3.453 1.00 0.00 O ATOM 1267 CB CYS A 87142.190 1.273 -2.438 1.00 0.00 C ATOM 1268 SG CYS A 87143.964 1.374 -2.773 1.00 0.00 S ATOM 1269 H CYS A 87141.256 2.032 -4.914 1.00 0.00 H ATOM 1270 HA CYS A 87141.807 -0.518 -3.544 1.00 0.00 H ATOM 1271 1HB CYS A 87141.806 2.283 -2.399 1.00 0.00 H ATOM 1272 2HB CYS A 87142.062 0.808 -1.472 1.00 0.00 H ATOM 1273 HG CYS A 87144.411 1.556 -1.943 1.00 0.00 H ATOM 1274 N ARG A 88139.607 -0.632 -2.286 1.00 0.00 N ATOM 1275 CA ARGA 88138.238 -0.829 -1.823 1.00 0.00 C ATOM 1276 C ARG A 88138.194 -0.971 -0.302 1.00 0.00 C

ATOM 1277 O ARG A 88139.090 -1.563 0.299 1.00 0.00 O ATOM 1278 CB ARG A 88137.630 -2.070 -2.481 1.00 0.00 C ATOM 1279 CG ARG A 88136.804 -1.758 -3.719 1.00 0.00 C ATOM 1280 CD ARG A 88135.321 -1.676 -3.394 1.00 0.00 C ATOM 1281 NE ARG A 88134.498 -2.278 -4.440 1.00 0.00 N ATOM 1282 CZ ARG A 88134.378 -3.590 -4.626 1.00 0.00 C ATOM 1283 NH1 ARG A 88135.026 -4.441 -3.839 1.00 0.00 N ATOM 1284 NH2 ARG A 88133.607 -4.054 -5.601 1.00 0.00 N ATOM 1285 H ARG A 88140.300 -1.268 -2.014 1.00 0.00 H ATOM 1286 HA ARG A 88137.663 0.038 -2.110 1.00 0.00 H ATOM 1287 1HB ARG A 88138.427 -2.739 -2.766 1.00 0.00 H ATOM 1288 2HB ARG A 88136.991 -2.567 -1.766 1.00 0.00 H ATOM 1289 1HG ARG A 88137.126 -0.811 -4.126 1.00 0.00 H ATOM 1290 2HG ARG A 88136.961 -2.537 -4.450 1.00 0.00 H ATOM 1291 1HD ARG A 88135.140 -2.193 -2.464 1.00 0.00 H ATOM 1292 2HD ARG A 88135.047 -0.636 -3.286 1.00 0.00 H ATOM 1293 HE ARG A 88134.008 -1.672 -5.035 1.00 0.00 H ATOM 1294 1HH1 ARG A 88135.608 -4.098 -3.103 1.00 0.00 H ATOM 1295 2HH1 ARG A 88134.932 -5.426 -3.984 1.00 0.00 H ATOM 1296 1HH2 ARG A 88133.117 -3.417 -6.195 1.00 0.00 H ATOM 1297 2HH2 ARG A 88133.518 -5.040 -5.741 1.00 0.00 H ATOM 1298 N PRO A 89137.145 -0.428 0.343 1.00 0.00 N ATOM 1299 CA PRO A 89136.992 -0.500 1.800 1.00 0.00 C ATOM 1300 C PRO A 89137.064 -1.933 2.319 1.00 0.00 C ATOM 1301 O PRO A 89136.429 -2.834 1.772 1.00 0.00 O ATOM 1302 CB PRO A 89135.600 0.087 2.047 1.00 0.00 C ATOM 1303 CG PRO A 89135,338 0.956 0.866 1.00 0.00 C ATOM 1304 CD PRO A 89136.029 0.296 -0.293 1.00 0.00 C ATOM 1305 HA PRO A 89137.735 0.101 2.305 1.00 0.00 H ATOM 1306 1HB PRO A 89134.878 -0.712 2.118 1.00 0.00 H ATOM 1307 2HB PRO A 89135.605 0.658 2.963 1.00 0.00 H

ATOM 1308 1HG PRO A 89134.275 1.018 0.684 1.00 0.00 H ATOM 1309 2HG PRO A 89135.748 1.940 1.037 1.00 0.00 H ATOM 1310 1HD PRO A 89135.359 -0.389 -0.793 1.00 0.00 H ATOM 1311 2HD PRO A 89136.397 1.039 -0.986 1.00 0.00 H ATOM 1312 N ASPA 90137.840 -2.134 3.379 1.00 0.00 N ATOM 1313 CA ASP A 90137.993 -3.457 3.973 1.00 0.00 C ATOM 1314 C ASPA 90137.169 -3.577 5.252 1.00 0.00 C ATOM 1315 O ASP A 90137.450 -2.910 6.248 1.00 0.00 O ATOM 1316 CB ASP A 90139.466 -3.738 4.273 1.00 0.00 C ATOM 1317 CG ASP A 90139.802 -5.214 4.188 1.00 0.00 C ATOM 1318 OD1 ASP A 90139.035 -5.962 3.546 1.00 0.00 O ATOM 1319 OD2 ASP A 90140.832 -5.623 4.765 1.00 0.00 O ATOM 1320 H ASPA 90138.319 -1.376 3.772 1.00 0.00 H ATOM 1321 HA ASPA 90137.634 -4.185 3.260 1.00 0.00 H ATOM 1322 1HB ASP A 90140.079 -3.207 3.561 1.00 0.00 H ATOM 1323 2HB ASP A 90139.697 -3.391 5.270 1.00 0.00 H ATOM 1324 N SER A 91136.152 -4.431 5.217 1.00 0.00 N ATOM 1325 CA SER A 91135.287 -4.638 6.373 1.00 0.00 C ATOM 1326 C SER A 91135.697 -5.889 7.143 1.00 0.00 C ATOM 1327 O SER A 91134.862 -6.551 7.760 1.00 0.00 O ATOM 1328 CB SER A 91133.828 -4.756 5.929 1.00 0.00 C ATOM 1329 OG SER A 91132.948 -4.280 6.933 1.00 0.00 O ATOM 1330 H SER A 91135.978 -4.935 4.394 1.00 0.00 H ATOM 1331 HA SER A 91135.389 -3.781 7.021 1.00 0.00 H ATOM 1332 1HB SER A 91133.678 -4.174 5.032 1.00 0.00 H ATOM 1333 2HB SER A 91133.598 -5.792 5.729 1.00 0.00 H ATOM 1334 HG SER A 91132.884 -3.323 6.875 1.00 0.00 H ATOM 1335 N ARG A 92136.986 -6.208 7.102 1.00 0.00 N ATOM 1336 CA ARG A 92137.506 -7.381 7.796 1.00 0.00 C ATOM 1337 C ARG A 92137.392 -7.216 9.308 1.00 0.00 C ATOM 1338 O ARG A 92137.237 -8.194 10.039 1.00 0.00 O

ATOM 1339 CB ARG A 92138.965 -7.625 7.407 1.00 0.00 C ATOM 1340 CG ARG A 92139.127 -8.507 6.179 1.00 0.00 C ATOM 1341 CD ARG A 92139.297 -9.967 6.561 1.00 0.00 C ATOM 1342 NE ARG A 92138.019 -10.606 6.867 1.00 0.00 N ATOM 1343 CZ ARG A 92137.901 -11.865 7.283 1.00 0.00 C ATOM 1344 NH1 ARG A 92138.978 -12.623 7.443 1.00 0.00 N ATOM 1345 NH2 ARG A 92136.700 -12.367 7.540 1.00 0.00 N ATOM 1346 H ARG A 92137.603 -5.642 6.593 1.00 0.00 H ATOM 1347 HA ARG A 92136.915 -8.232 7.494 1.00 0.00 H ATOM 1348 1HB ARG A 92139.435 -6.674 7.205 1.00 0.00 H ATOM 1349 2HB ARG A 92139.472 -8.100 8.234 1.00 0.00 H ATOM 1350 1HG ARG A 92138.250 -8.408 5.558 1.00 0.00 H ATOM 1351 2HG ARG A 92139.999 -8.183 5.629 1.00 0.00 H ATOM 1352 1HD ARG A 92139.761 -10.490 5.738 1.00 0.00 H ATOM 1353 2HD ARG A 92139.937 -10.027 7.430 1.00 0.00 H ATOM 1354 HE ARG A 92137.207 -10.069 6.758 1.00 0.00 H ATOM 1355 1HH1 ARG A 92139.885 -12.251 7.251 1.00 0.00 H ATOM 1356 2HH1 ARG A 92138.881 -13.568 7.756 1.00 0.00 H ATOM 1357 1HH2 ARG A 92135.885 -11.800 7.422 1.00 0.00 H ATOM 1358 2HH2 ARG A 92136.610 -13.314 7.852 1.00 0.00 H ATOM 1359 N PHE A 93137.469 -5.972 9.771 1.00 0.00 N ATOM 1360 CA PHE A 93137.374 -5.680 11.197 1.00 0.00 C ATOM 1361 C PHE A 93136.233 -4.710 11.482 1.00 0.00 C ATOM 1362 O PHE A 93136.297 -3.923 12.426 1.00 0.00 O ATOM 1363 CB PHE A 93138.694 -5.097 11.708 1.00 0.00 C ATOM 1364 CG PHE A 93139.869 -6.012 11.515 1.00 0.00 C ATOM 1365 CD1 PHE A 93140.315 -6.330 10.242 1.00 0.00 C ATOM 1366 CD2 PHE A 93140.529 -6.553 12.607 1.00 0.00 C ATOM 1367 CE1 PHE A 93141.396 -7.172 10.062 1.00 0.00 C ATOM 1368 CE2 PHE A 93141.611 -7.395 12.432 1.00 0.00 C ATOM 1369 CZ PHE A 93142.044 -7.705 11.158 1.00 0.00 C

ATOM 1370 H PHE A 93137.593 -5.233 9.140 1.00 0.00 H ATOM 1371 HA PHE A 93137.179 -6.609 11.713 1.00 0.00 H ATOM 1372 1HB PHE A 93138.900 -4.177 11.182 1.00 0.00 H ATOM 1373 2HB PHE A 93138.602 -4.889 12.764 1.00 0.00 H ATOM 1374 HD1 PHE A 93139.808 -5.914 9.384 1.00 0.00 H ATOM 1375 HD2 PHE A 93140.191 -6.311 13.603 1.00 0.00 H ATOM 1376 HE1 PHE A 93141.732 -7.413 9.064 1.00 0.00 H ATOM 1377 HE2 PHE A 93142.116 -7.810 13.292 1.00 0.00 H ATOM 1378 HZ PHE A 93142.890 -8.363 11.020 1.00 0.00 H ATOM 1379 N ALA A 94135.189 -4.773 10.663 1.00 0.00 N ATOM 1380 CA ALAA 94134.033 -3.900 10.832 1.00 0.00 C ATOM 1381 C. ALA A 94133.305 -4.199 12.137 1.00 0.00 C ATOM 1382 O ALA A 94133.012 -5.354 12.445 1.00 0.00 O ATOM 1383 CB ALA A 94133.085 -4.045 9.650 1.00 0.00 C ATOM 1384 H ALAA 94135.193 -5.422 9.929 1.00 0.00 H ATOM 1385 HA ALA A 94134.388 -2.879 10.856 1.00 0.00 H ATOM 1386 1HB ALA A 94133.208 -5.023 9.210 1.00 0.00 H ATOM 1387 2HB ALA A 94133.309 -3.287 8.914 1.00 0.00 H ATOM 1388 3HB ALA A 94132.067 -3.928 9.990 1.00 0.00 H ATOM 1389 N SER A 95133.013 -3.150 12.901 1.00 0.00 N ATOM 1390 CA SER A 95132.317 -3.302 14.173 1.00 0.00 C ATOM 1391 C SER A 95130.916 -3.866 13.962 1.00 0.00 C ATOM 1392 O SER A 95130.374 -3.811 12.859 1.00 0.00 O ATOM 1393 CB SER A 95132.236 -1.957 14.897 1.00 0.00 C ATOM 1394 OG SER A 95132.416 -2.118 16.294 1.00 0.00 O ATOM 1395 H SER A 95133.272 -2.255 12.601 1.00 0.00 H ATOM 1396 HA SER A 95132.883 -3.993 14.780 1.00 0.00 H ATOM 1397 1HB SER A 95133.008 -1.301 14.522 1.00 0.00 H ATOM 1398 2HB SER A 95131.268 -1.513 14.719 1.00 0.00 H ATOM 1399 HG SER A 95133.342 -2.288 16.481 1.00 0.00 H ATOM 1400 N LEU A 96130.335 -4.410 15.026 1.00 0.00 N

ATOM 1401 CA LEU A 96128.997 -4.986 14.956 1.00 0.00 C ATOM 1402 C LEU A 96128.036 -4.263 15.895 1.00 0.00 C ATOM 1403 O LEUA 96126.868 -4.055 15.564 1.00 0.00 O ATOM 1404 CB LEU A 96129.042 -6.476 15.303 1.00 0.00 C ATOM 1405 CG LEU A 96128.119 -7.363 14.466 1.00 0.00 C ATOM 1406 CD1 LEU A 96128.828 -7.831 13.204 1.00 0.00 C ATOM 1407 CD2 LEU A 96127.642 -8.555 15.284 1.00 0.00 C ATOM 1408 H LEU A 96130.818 -4.426 15.879 1.00 0.00 H ATOM 1409 HA LEUA 96128.642 -4.872 13.944 1.00 0.00 H ATOM 1410 1HB LEU A 96130.057 -6.823 15.170 1.00 0.00 H ATOM 1411 2HB LEU A 96128.772 -6.592 16.341 1.00 0.00 H ATOM 1412 HG LEUA 96127.252 -6.792 14.168 1.00 0.00 H ATOM 1413 1HD1 LEU A 96129.233 -8.820 13.364 1.00 0.00 H ATOM 1414 2HD1 LEU A 96129.629 -7.148 12.967 1.00 0.00 H ATOM 1415 3HD1 LEU A 96128.124 -7.860 12.385 1.00 0.00 H ATOM 1416 1HD2 LEU A 96127.529 -9.413 14.639 1.00 0.00 H ATOM 1417 2HD2 LEU A 96126.691 -8.319 15.740 1.00 0.00 H ATOM 1418 3HD2 LEU A 96128.365 -8.775 16.054 1.00 0.00 H ATOM 1419 N GLN A 97128.533 -3.884 17.066 1.00 0.00 N ATOM 1420 CA GLN A 97127.716 -3.187 18.053 1.00 0.00 C ATOM 1421 C GLN A 97127.507 -1.726 17.658 1.00 0.00 C ATOM 1422 O GLN A 97126.376 -1.290 17.445 1.00 0.00 O ATOM 1423 CB GLN A 97128.369 -3.269 19.436 1.00 0.00 C ATOM 1424 CG GLN A 97127.712 -4.284 20.358 1.00 0.00 C ATOM 1425 CD GLN A 97128.057 -5.715 19.990 1.00 0.00 C ATOM 1426 OE1 GLN A 97129.195 -6.154 20.161 1.00 0.00 O ATOM 1427 NE2 GLN A 97127.075 -6.449 19.483 1.00 0.00 N ATOM 1428 H GLN A 97129.470 -4.080 17.272 1.00 0.00 H ATOM 1429 HA GLN A 97126.755 -3.677 18.090 1.00 0.00 H ATOM 1430 1HB GLN A 97129.406 -3.543 19.315 1.00 0.00 H ATOM 1431 2HB GLN A 97128.313 -2.299 19.908 1.00 0.00 H

ATOM 1432 1HG GLN A 97128.042 -4.100 21.370 1.00 0.00 H ATOM 1433 2HG GLN A 97126.641 -4.162 20.301 1.00 0.00 H ATOM 1434 1HE2 GLN A 97126.193 -6.033 19.375 1.00 0.00 H ATOM 1435 2HE2 GLN A 97127.270 -7.377 19.237 1.00 0.00 H ATOM 1436 N PRO A 98128.598 -0.947 17.556 1.00 0.00 N ATOM 1437 CA PRO A 98128.523 0.469 17.186 1.00 0.00 C ATOM 1438 C PRO A 98128.237 0.667 15.701 1.00 0.00 C ATOM 1439 O PRO A 98128.153 -0.297 14.942 1.00 0.00 O ATOM 1440 CB PRO A 98129.913 0.996 17.538 1.00 0.00 C ATOM 1441 CG PRO A 98130.809 -0.185 17.397 1.00 0.00 C ATOM 1442 CD PRO A 98129.988 -1.383 17.795 1.00 0.00 C ATOM 1443 HA PRO A 98127.778 0.992 17.768 1.00 0.00 H ATOM 1444 1HB PRO A 98130.186 1.786 16.853 1.00 0.00 H ATOM 1445 2HB PRO A 98129.914 1.372 18.551 1.00 0.00 H ATOM 1446 1HG PRO A 98131.134 -0.278 16.370 1.00 0.00 H ATOM 1447 2HG PRO A 98131.661 -0.081 18.052 1.00 0.00 H ATOM 1448 1HD PRO A 98130.236 -2.233 17.175 1.00 0.00 H ATOM 1449 2HD PRO A 98130.144 -1.617 18.837 1.00 0.00 H ATOM 1450 N SER A 99128.090 1.923 15.295 1.00 0.00 N ATOM 1451 CA SER A 99127.813 2.249 13.901 1.00 0.00 C ATOM 1452 C SER A 99126.511 1.603 13.438 1.00 0.00 C ATOM 1453 O SER A 99125.885 0.845 14.180 1.00 0.00 O ATOM 1454 CB SER A 99128.968 1.789 13.009 1.00 0.00 C ATOM 1455 OG SER A 99129.924 2.821 12.839 1.00 0.00 O ATOM 1456 H SER A 99128.168 2.649 15.948 1.00 0.00 H ATOM 1457 HA SER A 99127.716 3.321 13.824 1.00 0.00 H ATOM 1458 1HB SER A 99129.453 0.937 13.463 1.00 0.00 H ATOM 1459 2HB SER A 99128.582 1.509 12.039 1.00 0.00 H ATOM 1460 HG SER A 99129.542 3.530 12.318 1.00 0.00 H ATOM 1461 N GLY A 100126.108 1.908 12.209 1.00 0.00 N ATOM 1462 CA GLY A 100124.883 1.349 11.670 1.00 0.00 C

ATOM 1463 C GLY A 100124.519 1.941 10.322 1.00 0.00 C ATOM 1464 O GLY A 100123.482 2.592 10.188 1.00 0.00 O ATOM 1465 H GLY A 100126.648 2.518 11.664 1.00 0.00 H ATOM 1466 1HA GLY A 100125.005 0.282 11.561 1.00 0.00 H ATOM 1467 2HA GLY A 100124.078 1.540 12.364 1.00 0.00 H ATOM 1468 N PRO A 101125.359 1.731 9.293 1.00 0.00 N ATOM 1469 CA PRO A 101125.107 2.256 7.947 1.00 0.00 C ATOM 1470 C PRO A 101123.718 1.890 7.433 1.00 0.00 C ATOM 1471 O PRO A 101122.980 2.747 6.947 1.00 0.00 O ATOM 1472 CB PRO A 101126.186 1.585 7.096 1.00 0.00 C ATOM 1473 CG PRO A 101127.285 1.275 8.051 1.00 0.00 C ATOM 1474 CD PRO A 101126.618 0.967 9.363 1.00 0.00 C ATOM 1475 HA PRO A 101125.231 3.328 7.912 1.00 0.00 H ATOM 1476 1HB PRO A 101125.786 0.687 6.645 1.00 0.00 H ATOM 1477 2HB PRO A 101126.515 2.265 6.324 1.00 0.00 H ATOM 1478 1HG PRO A 101127.842 0.418 7.703 1.00 0.00 H ATOM 1479 2HG PRO A 101127.935 2.131 8.153 1.00 0.00 H ATOM 1480 1HD PRO A 101126.423 -0.092 9.447 1.00 0.00 H ATOM 1481 2HD PRO A 101127.230 1.306 10.185 1.00 0.00 H ATOM 1482 N SER A 102123.369 0.613 7.545 1.00 0.00 N ATOM 1483 CA SER A 102122.069 0.133 7.093 1.00 0.00 C ATOM 1484 C SER A 102121.100 -0.001 8.263 1.00 0.00 C ATOM 1485 O SER A 102121.516 -0.103 9.417 1.00 0.00 O ATOM 1486 CB SER A 102122.218 -1.213 6.382 1.00 0.00 C ATOM 1487 OG SER A 102123.120 -1.118 5.293 1.00 0.00 O ATOM 1488 H SER A 102124.001 -0.023 7.942 1.00 0.00 H ATOM 1489 HA SER A 102121.674 0.857 6.395 1.00 0.00 H ATOM 1490 1HB SER A 102122.592 -1.947 7.079 1.00 0.00 H ATOM 1491 2HB SER A 102121.255 -1.529 6.008 1.00 0.00 H ATOM 1492 HG SER A 102124.020 -1.072 5.626 1.00 0.00 H ATOM 1493 N SER A 103119.807 -0.001 7.957 1.00 0.00 N

ATOM 1494 CA SER A 103118.779 -0.124 8.984 1.00 0.00 C ATOM 1495 C SER A 103117.615 -0.978 8.491 1.00 0.00 C ATOM 1496 O SER A 103117.578 -1.380 7.327 1.00 0.00 O ATOM 1497 CB SER A 103118.273 1.260 9.396 1.00 0.00 C ATOM 1498 OG SER A 103119.008 1.766 10.496 1.00 0.00 O ATOM 1499 H SER A 103119.538 0.082 7.018 1.00 0.00 H ATOM 1500 HA SER A 103119.224 -0.605 9.842 1.00 0.00 H ATOM 1501 1HB SER A 103118.378 1.941 8.566 1.00 0.00 H ATOM 1502 2HB SER A 103117.231 1.191 9.675 1.00 0.00 H ATOM 1503 HG SER A 103118.404 2.011 11.200 1.00 0.00 H ATOM 1504 N GLY A 104116.668 -1.250 9.382 1.00 0.00 N ATOM 1505 CA GLY A 104115.517 -2.054 9.017 1.00 0.00 C ATOM 1506 C GLY A 104115.849 -3.530 8.912 1.00 0.00 C ATOM 1507 O GLY A 104116.578 -3.908 7.971 1.00 0.00 O ATOM 1508 OXT GLY A 104115.381 -4.306 9.770 1.00 0.00 O ATOM 1509 H GLY A 104116.751 -0.902 10.294 1.00 0.00 H ATOM 1510 1HA GLY A 104114.748 -1.923 9.764 1.00 0.00 H ATOM 1511 2HA GLY A 104115.140 -1.712 8.064 1.00 0.00 H TER 1512 GLY A 104 **ENDMDL**

Three-Dimensional Structure Coordinate Table 11

ATOM 1 N GLYA 1115.866 3.091 -14.965 1.00 0.00 N ATOM 2 CA GLYA 1115.463 4.481 -15.313 1.00 0.00 C ATOM 3 C GLYA 1114.748 5.178 -14.173 1.00 0.00 C ATOM 4 O GLYA 1115.178 6.239 -13.718 1.00 0.00 O ATOM 5 1H GLYA 1115.734 2.465 -15.785 1.00 0.00 H ATOM 6 2H GLYA 1115.288 2.737 -14.177 1.00 0.00 H ATOM 7 3H GLYA 1116.867 3.069 -14.684 1.00 0.00 H ATOM 8 1HA GLYA 1116.347 5.047 -15.568 1.00 0.00 H ATOM 9 2HA GLYA 1114.807 4.450 -16.170 1.00 0.00 H ATOM10 N SER A 2113.654 4.584 -13.710 1.00 0.00 N ATOM11 CA SER A 2112.877 5.154 -12.617 1.00 0.00 C ATOM12 C SER A 2113.073 4.352 -11.334 1.00 0.00 C ATOM13 O SER A 2112.499 3.275 -11.170 1.00 0.00 O ATOM14 CB SER A 2111.393 5.196 -12.984 1.00 0.00 C ATOM15 OG SER A 2110.991 3.994 -13.621 1.00 0.00 O ATOM16 H SER A 2113.361 3.739 -14.114 1.00 0.00 H ATOM17 HA SER A 2113.225 6.163 -12.454 1.00 0.00 H ATOM18 1HB SER A 2110.805 5.327 -12.088 1.00 0.00 H ATOM19 2HB SER A 2111.213 6.021 -13.656 1.00 0.00 H ATOM20 HG SER A 2110.163 4.140 -14.085 1.00 0.00 H ATOM21 N SER A 3113.885 4.885 -10.428 1.00 0.00 N ATOM22 CA SER A 3114.158 4.219 -9.160 1.00 0.00 C ATOM23 C SER A 3114.271 5.234 -8.026 1.00 0.00 C ATOM24 O SER A 3115.013 5.026 -7.066 1.00 0.00 O ATOM25 CB SER A 3115.444 3.398 -9.257 1.00 0.00 C ATOM26 OG SER A 3116.585 4.238 -9.267 1.00 0.00 O ATOM27 H SER A 3114.313 5.746 -10.617 1.00 0.00 H ATOM28 HA SER A 3113.332 3.555 -8.951 1.00 0.00 H ATOM29 1HB SER A 3115.510 2.733 -8.407 1.00 0.00 H ATOM30 2HB SER A 3115.431 2.817 -10.168 1.00 0.00 H ATOM31 HG SER A 3117.076 4.121 -8.450 1.00 0.00 H ATOM32 N GLY A 4113.532 6.331 -8.144 1.00 0.00 N ATOM33 CA GLY A 4113.564 7.361 -7.124 1.00 0.00 C ATOM34 C GLY A 4114.925 8.018 -7.006 1.00 0.00 C ATOM35 O GLY A 4115.618 8.209 -8.005 1.00 0.00 O ATOM36 H GLY A 4112.959 6.442 -8.932 1.00 0.00 H ATOM37 1HA GLY A 4112.831 8.116 -7.366 1.00 0.00 H ATOM38 2HA GLY A 4113.308 6.918 -6.172 1.00 0.00 H ATOM39 N SER A 5115.308 8.367 -5.781 1.00 0.00 N ATOM40 CA SER A 5116.595 9.007 -5.536 1.00 0.00 C

ATOM41 C SER A 5117.744 8.053 -5.842 1.00 0.00 C ATOM42 O SER A 5117.532 6.947 -6.339 1.00 0.00 O ATOM43 CB SER A 5116.683 9.483 -4.086 1.00 0.00 C ATOM44 OG SER A 5116.895 8.395 -3.204 1.00 0.00 O ATOM45 H SER A 5114.711 8.189 -5.025 1.00 0.00 H ATOM46 HA SER A 5116.669 9.863 -6.192 1.00 0.00 H ATOM47 1HB SER A 5117.505 10.176 -3.985 1.00 0.00 H ATOM48 2HB SER A 5115.761 9.977 -3.814 1.00 0.00 H ATOM49 HG SER A 5117.254 8.719 -2.374 1.00 0.00 H ATOM50 N SER A 6118.964 8.488 -5.541 1.00 0.00 N ATOM51 CA SER A 6120.148 7.672 -5.783 1.00 0.00 C ATOM52 C SER A 6121.050 7.644 -4.553 1.00 0.00 C ATOM53 O SER A 6120.819 8.368 -3.585 1.00 0.00 O ATOM54 CB SER A 6120.925 8.209 -6.987 1.00 0.00 C ATOM55 OG SER A 6120.330 7.794 -8.204 1.00 0.00 O ATOM56 H SER A 6119.070 9.379 -5.147 1.00 0.00 H ATOM57 HA SER A 6119.819 6.667 -5.998 1.00 0.00 H ATOM58 1HB SER A 6120.934 9.288 -6.955 1.00 0.00 H ATOM59 2HB SER A 6121.940 7.839 -6.952 1.00 0.00 H ATOM60 HG SER A 6119.960 8.556 -8.656 1.00 0.00 H ATOM61 N GLY A 7122.078 6.802 -4.599 1.00 0.00 N ATOM62 CA GLY A 7122.998 6.694 -3.483 1.00 0.00 C ATOM63 C GLY A 7124.358 7.292 -3.792 1.00 0.00 C ATOM64 O GLY A 7125.374 6.600 -3.734 1.00 0.00 O ATOM65 H GLY A 7122.211 6.250 -5.398 1.00 0.00 H ATOM66 1HA GLY A 7122.577 7.208 -2.631 1.00 0.00 H ATOM67 2HA GLY A 7123.125 5.651 -3.234 1.00 0.00 H ATOM68 N LEUA 8124.375 8.579 -4.121 1.00 0.00 N ATOM69 CA LEU A 8125.618 9.269 -4.441 1.00 0.00 C ATOM70 C LEUA 8126.203 9.939 -3.201 1.00 0.00 C ATOM71 O LEUA 8125.836 11.063 -2.860 1.00 0.00 O

ATOM72 CB LEU A 8125,382 10.312 -5.534 1.00 0.00 C ATOM73 CG LEU A 8125.496 9.786 -6.966 1.00 0.00 C ATOM74 CD1 LEU A 8124.571 10.560 -7.895 1.00 0.00 C ATOM75 CD2 LEU A 8126.936 9.874 -7.451 1.00 0.00 C ATOM76 H LEUA 8123.530 9.077 -4.149 1.00 0.00 H ATOM77 HA LEU A 8126.321 8.535 -4.804 1.00 0.00 H ATOM78 1HB LEU A 8124.390 10.723 -5.402 1.00 0.00 H ATOM79 2HB LEU A 8126.102 11.106 -5.409 1.00 0.00 H ATOM80 HG LEU A 8125.198 8.749 -6.987 1.00 0.00 H ATOM81 1HD1 LEU A 8124.613 10.130 -8.884 1.00 0.00 H ATOM82 2HD1 LEU A 8124.884 11.592 -7.936 1.00 0.00 H ATOM83 3HD1 LEU A 8123.559 10.504 -7.521 1.00 0.00 H ATOM84 1HD2 LEU A 8127.427 10.708 -6.971 1.00 0.00 H ATOM85 2HD2 LEU A 8126.946 10.018 -8.521 1.00 0.00 H ATOM86 3HD2 LEU A 8127.454 8.960 -7.205 1.00 0.00 H ATOM87 N ALAA 9127.114 9.241 -2.531 1.00 0.00 N ATOM88 CA ALA A 9127.749 9.768 -1.330 1.00 0.00 C ATOM89 C ALA A 9129.268 9.670 -1.424 1.00 0.00 C ATOM90 O ALAA 9129.869 8.705 -0.951 1.00 0.00 O ATOM91 CB ALA A 9127.246 9.027 -0.100 1.00 0.00 C ATOM92 H ALAA 9127.366 8.351 -2.854 1.00 0.00 H ATOM93 HA ALA A 9127.471 10.807 -1.234 1.00 0.00 H ATOM94 1HB ALA A 9127.736 8.068 -0.032 1.00 0.00 H ATOM95 2HB ALA A 9126.179 8.883 -0.179 1.00 0.00 H ATOM96 3HB ALA A 9127.466 9.607 0.785 1.00 0.00 H ATOM97 N MET A 10129.884 10.676 -2.036 1.00 0.00 N ATOM98 CA MET A 10131.333 10.704 -2.192 1.00 0.00 C ATOM99 C MET A 10131.803 12.075 -2.673 1.00 0.00 C ATOM 100 O MET A 10132.290 12.217 -3.796 1.00 0.00 O 101 CB MET A 10131.781 9.621 -3.177 1.00 0.00 C ATOM ATOM 102 CG MET A 10131.011 9.633 -4.487 1.00 0.00 C

103 SD MET A 10132.039 9.194 -5.902 1.00 0.00 S **ATOM** 104 CE MET A 10131.756 10.599 -6.975 1.00 0.00 C 105 H META 10129.350 11.418 -2.392 1.00 0.00 H **ATOM** ATOM 106 HA MET A 10131.774 10.503 -1.227 1.00 0.00 H 107 1HB MET A 10132.829 9.764 -3.399 1.00 0.00 H ATOM 108 2HB MET A 10131.649 8.654 -2.715 1.00 0.00 H ATOM 109 1HG MET A 10130.198 8.925 -4.418 1.00 0.00 H **ATOM ATOM** 110 2HG META 10130.610 10.624 -4.645 1.00 0.00 H **ATOM** 111 1HE MET A 10132.698 10.931 -7.388 1.00 0.00 H 112 2HE MET A 10131.308 11.401 -6.408 1.00 0.00 H **ATOM** 113 3HE MET A 10131.094 10.311 -7.778 1.00 0.00 H ATOM 114 N PRO A 11131.663 13.108 -1.824 1.00 0.00 N **ATOM** 115 CA PRO A 11132.074 14.473 -2.167 1.00 0.00 C ATOM 116 C PROA 11133.551 14.563 -2.551 1.00 0.00 C **ATOM** 117 O PRO A 11133.898 15.181 -3.558 1.00 0.00 O **ATOM ATOM** 118 CB PRO A 11131.805 15.271 -0.886 1.00 0.00 C **ATOM** 119 CG PRO A 11130.807 14.463 -0.129 1.00 0.00 C 120 CD PRO A 11131.093 13.028 -0.468 1.00 0.00 C **ATOM** 121 HA PRO A 11131.475 14.872 -2.972 1.00 0.00 H **ATOM ATOM** 122 1HB PRO A 11132.723 15.387 -0.331 1.00 0.00 H **ATOM** 123 2HB PRO A 11131.410 16.243 -1.142 1.00 0.00 H 124 1HG PRO A 11130.929 14.629 0.931 1.00 0.00 H ATOM 125 2HG PRO A 11129.808 14.729 -0.439 1.00 0.00 H **ATOM** 126 1HD PRO A 11131.806 12.609 0.227 1.00 0.00 H ATOM 127 2HD PRO A 11130.180 12.450 -0.468 1.00 0.00 H **ATOM** 128 N PRO A 12134.450 13.949 -1.756 1.00 0.00 N ATOM 129 CA PRO A 12135.886 13.974 -2.032 1.00 0.00 C ATOM 130 C PRO A 12136.292 12.960 -3.095 1.00 0.00 C ATOM 131 O PROA 12137.238 13.182 -3.852 1.00 0.00 O ATOM 132 CB PRO A 12136.500 13.610 -0.682 1.00 0.00 C **ATOM** 133 CG PRO A 12135.490 12.722 -0.040 1.00 0.00 C ATOM

134 CD PRO A 12134.140 13.185 -0.528 1.00 0.00 C **ATOM** 135 HA PRO A 12136.216 14.959 -2.328 1.00 0.00 H **ATOM ATOM** 136 1HB PRO A 12137.438 13.099 -0.837 1.00 0.00 H 137 2HB PRO A 12136.662 14.507 -0.103 1.00 0.00 H ATOM **ATOM** 138 1HG PRO A 12135.663 11.698 -0.336 1.00 0.00 H 139 2HG PRO A 12135.551 12.816 1.034 1.00 0.00 H ATOM **ATOM** 140 1HD PRO A 12133.514 12.336 -0.753 1.00 0.00 H 141 2HD PRO A 12133.670 13.816 0.211 1.00 0.00 H **ATOM** 142 N GLYA 13135.571 11.845 -3.148 1.00 0.00 N **ATOM ATOM** 143 CA GLY A 13135.870 10.813 -4.124 1.00 0.00 C 144 C GLY A 13135.828 9.420 -3.526 1.00 0.00 C **ATOM ATOM** 145 O GLYA 13135.130 9.182 -2.540 1.00 0.00 O 146 H GLY A 13134.829 11.722 -2.520 1.00 0.00 H **ATOM** 147 1HA GLY A 13135.150 10.871 -4.926 1.00 0.00 H **ATOM** 148 2HA GLY A 13136.857 10.990 -4.526 1.00 0.00 H **ATOM** 149 N ASNA 14136.576 8.499 -4.124 1.00 0.00 N **ATOM** 150 CA ASN A 14136.621 7.122 -3.645 1.00 0.00 C ATOM 151 C ASN A 14135.237 6.483 -3.698 1.00 0.00 C **ATOM** 152 O ASNA 14134.268 7.110 -4.126 1.00 0.00 O ATOM 153 CB ASN A 14137.162 7.075 -2.215 1.00 0.00 C **ATOM** 154 CG ASN A 14138.589 7.579 -2.120 1.00 0.00 C **ATOM** 155 OD1 ASN A 14139.533 6.793 -2.045 1.00 0.00 O **ATOM** 156 ND2 ASN A 14138.752 8.897 -2.121 1.00 0.00 N **ATOM** 157 H ASNA 14137.110 8.751 -4.906 1.00 0.00 H **ATOM** 158 HA ASN A 14137.286 6.568 -4.290 1.00 0.00 H **ATOM** 159 1HB ASN A 14136.541 7.689 -1.581 1.00 0.00 H **ATOM** 160 2HB ASN A 14137.135 6.055 -1.860 1.00 0.00 H **ATOM** 161 1HD2 ASN A 14137.954 9.462 -2.183 1.00 0.00 H **ATOM** 162 2HD2 ASN A 14139.665 9.250 -2.062 1.00 0.00 H **ATOM** 163 N SER A 15135.153 5.230 -3.261 1.00 0.00 N **ATOM** 164 CA SER A 15133.889 4.505 -3.259 1.00 0.00 C ATOM

165 C SER A 15133.091 4.806 -1.995 1.00 0.00 C ATOM 166 O SER A 15131.921 5.185 -2.062 1.00 0.00 O ATOM **ATOM** 167 CB SER A 15134.139 3.000 -3.372 1.00 0.00 C 168 OG SER A 15135.400 2.651 -2.828 1.00 0.00 O ATOM 169 H SER A 15135.961 4.783 -2.933 1.00 0.00 H **ATOM** 170 HA SER A 15133.318 4.831 -4.116 1.00 0.00 H ATOM **ATOM** 171 1HB SER A 15133.369 2.468 -2.834 1.00 0.00 H 172 2HB SER A 15134.117 2.710 -4.413 1.00 0.00 H **ATOM** 173 HG SER A 15135.437 1.701 -2.690 1.00 0.00 H **ATOM ATOM** 174 N HIS A 16133.731 4.634 -0.843 1.00 0.00 N 175 CA HIS A 16133.082 4.888 0.438 1.00 0.00 C ATOM 176 C HIS A 16133.911 5.845 1.287 1.00 0.00 C **ATOM** 177 O HIS A 16133.495 6.971 1.559 1.00 0.00 O ATOM 178 CB HIS A 16132.862 3.573 1.192 1.00 0.00 C **ATOM** 179 CG HIS A 16131.453 3.072 1.121 1.00 0.00 C ATOM 180 ND1 HIS A 16130.429 3.599 1.878 1.00 0.00 N **ATOM** 181 CD2 HIS A 16130.900 2.083 0.378 1.00 0.00 C ATOM 182 CE1 HIS A 16129.306 2.957 1.605 1.00 0.00 C **ATOM** 183 NE2 HIS A 16129.566 2.033 0.697 1.00 0.00 N ATOM 184 H HIS A 16134.662 4.329 -0.855 1.00 0.00 H ATOM 185 HA HIS A 16132.122 5.341 0.239 1.00 0.00 H **ATOM** 186 1HB HIS A 16133.506 2.814 0.771 1.00 0.00 H ATOM 187 2HB HIS A 16133.115 3.715 2.233 1.00 0.00 H ATOM 188 HD1 HIS A 16130.511 4.334 2.522 1.00 0.00 H ATOM 189 HD2 HIS A 16131.414 1.452 -0.334 1.00 0.00 H ATOM 190 HE1 HIS A 16128.341 3.155 2.047 1.00 0.00 H ATOM 191 HE2 HIS A 16128.929 1.360 0.379 1.00 0.00 H **ATOM** 192 N GLYA 17135.088 5.388 1.705 1.00 0.00 N ATOM 193 CA GLY A 17135.958 6.216 2.519 1.00 0.00 C **ATOM** 194 C GLY A 17137.253 5.516 2.881 1.00 0.00 C ATOM ATOM 195 O GLY A 17137.419 5.048 4.007 1.00 0.00 O

ATOM 196 H GLYA 17135.368 4.483 1.458 1.00 0.00 H 197 1HA GLY A 17136.190 7.120 1.975 1.00 0.00 H **ATOM** 198 2HA GLY A 17135.438 6.480 3.428 1.00 0.00 H **ATOM** 199 N LEUA 18138.173 5.445 1.924 1.00 0.00 N **ATOM** 200 CA LEUA 18139.459 4.796 2.147 1.00 0.00 C ATOM 201 C LEUA 18140.511 5.811 2.583 1.00 0.00 C **ATOM** 202 O LEUA 18141.018 6.584 1.770 1.00 0.00 O **ATOM** 203 CB LEU A 18139.920 4.080 0.876 1.00 0.00 C **ATOM** 204 CG LEU A 18138.891 3.132 0.258 1.00 0.00 C **ATOM** 205 CD1 LEU A 18139.244 2.832 -1.190 1.00 0.00 C **ATOM** 206 CD2 LEU A 18138.800 1.846 1.066 1.00 0.00 C ATOM 207 H LEUA 18137.981 5.839 1.046 1.00 0.00 H **ATOM** 208 HA LEU A 18139.330 4.068 2.934 1.00 0.00 H ATOM 209 1HB LEU A 18140.178 4.828 0.140 1.00 0.00 H **ATOM** 210 2HB LEU A 18140.805 3.510 1.110 1.00 0.00 H **ATOM** 211 HG LEUA 18137.920 3.607 0.273 1.00 0.00 H **ATOM** 212 1HD1 LEU A 18140.311 2.936 -1.330 1.00 0.00 H **ATOM** 213 2HD1 LEU A 18138.727 3.523 -1.838 1.00 0.00 H ATOM 214 3HD1 LEU A 18138.947 1.822 -1.430 1.00 0.00 H **ATOM** 215 1HD2 LEU A 18138.009 1.934 1.795 1.00 0.00 H ATOM **ATOM** 216 2HD2 LEU A 18139.738 1.672 1.571 1.00 0.00 H 217 3HD2 LEU A 18138.589 1.020 0.403 1.00 0.00 H **ATOM ATOM** 218 N GLUA 19140.837 5.801 3.872 1.00 0.00 N 219 CA GLUA 19141.830 6.719 4.417 1.00 0.00 C ATOM 220 C GLUA 19142.803 5.984 5.335 1.00 0.00 C **ATOM** 221 O GLUA 19142.669 4.782 5.563 1.00 0.00 O **ATOM** 222 CB GLUA 19141.144 7.851 5.183 1.00 0.00 C **ATOM** 223 CG GLUA 19140.169 7.365 6.242 1.00 0.00 C ATOM 224 CD GLUA 19139.068 8.368 6.526 1.00 0.00 C **ATOM** 225 OE1 GLU A 19139.317 9.321 7.292 1.00 0.00 O ATOM ATOM 226 OE2 GLU A 19137.956 8.198 5.981 1.00 0.00 O

227 H GLUA 19140.399 5.160 4.471 1.00 0.00 H 228 HA GLU A 19142.383 7.138 3.590 1.00 0.00 H 229 1HB GLUA 19141.899 8.451 5.668 1.00 0.00 H ATOM 230 2HB GLU A 19140.602 8.467 4.481 1.00 0.00 H 231 1HG GLUA 19139.717 6.445 5.903 1.00 0.00 H **ATOM** 232 2HG GLUA 19140.713 7.181 7.157 1.00 0.00 H ATOM 233 N VALA 20143.782 6.716 5.858 1.00 0.00 N **ATOM** 234 CA VALA 20144.777 6.134 6.751 1.00 0.00 C **ATOM** 235 C VALA 20144.121 5.557 8.000 1.00 0.00 C ATOM 236 O VALA 20143.192 6.145 8.554 1.00 0.00 O **ATOM** 237 CB VAL A 20145.832 7.173 7.171 1.00 0.00 C ATOM 238 CG1 VAL A 20146.959 6.510 7.947 1.00 0.00 C **ATOM** 239 CG2 VAL A 20146.373 7.907 5.954 1.00 0.00 C ATOM 240 H VALA 20143.837 7.669 5.638 1.00 0.00 H **ATOM** 241 HA VALA 20145.277 5.338 6.219 1.00 0.00 H ATOM 242 HB VALA 20145.357 7.897 7.819 1.00 0.00 H **ATOM** 243 1HG1 VAL A 20147.274 5.615 7.430 1.00 0.00 H ATOM 244 2HG1 VAL A 20146.611 6.249 8.936 1.00 0.00 H ATOM 245 3HG1 VAL A 20147.792 7.192 8.026 1.00 0.00 H ATOM 246 1HG2 VAL A 20146.325 7.258 5.091 1.00 0.00 H **ATOM ATOM** 247 2HG2 VAL A 20147.398 8.194 6.132 1.00 0.00 H 248 3HG2 VAL A 20145.778 8.790 5.772 1.00 0.00 H 249 N GLY A 21144.611 4.402 8.440 1.00 0.00 N **ATOM** 250 CA GLY A 21144.060 3.766 9.623 1.00 0.00 C ATOM 251 C GLY A 21143.052 2.684 9.282 1.00 0.00 C **ATOM** 252 O GLY A 21142.879 1.729 10.039 1.00 0.00 O ATOM 253 H GLYA 21145.351 3.979 7.959 1.00 0.00 H ATOM 254 1HA GLY A 21144.867 3.325 10.189 1.00 0.00 H **ATOM** 255 2HA GLY A 21143.575 4.516 10.229 1.00 0.00 H **ATOM** 256 N SER A 22142.387 2.835 8.142 1.00 0.00 N ATOM ATOM 257 CA SER A 22141.391 1.865 7.703 1.00 0.00 C

258 C SER A 22142.020 0.815 6.794 1.00 0.00 C ATOM ATOM 259 O SER A 22143.073 1.045 6.198 1.00 0.00 O **ATOM** 260 CB SER A 22140.248 2.570 6.974 1.00 0.00 C 261 OG SER A 22139.563 3.461 7.837 1.00 0.00 O ATOM 262 H SER A 22142.570 3.619 7.582 1.00 0.00 H **ATOM** ATOM 263 HA SER A 22140.998 1.374 8.581 1.00 0.00 H 264 1HB SER A 22140.646 3.131 6.142 1.00 0.00 H 265 2HB SER A 22139.548 1.833 6.608 1.00 0.00 H **ATOM** 266 HG SER A 22138.635 3.220 7.876 1.00 0.00 H **ATOM ATOM** 267 N LEUA 23141.368 -0.338 6.690 1.00 0.00 N **ATOM** 268 CA LEU A 23141.863 -1.425 5.852 1.00 0.00 C **ATOM** 269 C LEUA 23141.319 -1.307 4.431 1.00 0.00 C 270 O LEUA 23140.227 -0.781 4.216 1.00 0.00 O **ATOM** 271 CB LEU A 23141.473 -2.777 6.451 1.00 0.00 C **ATOM** 272 CG LEU A 23142.132 -3.107 7.790 1.00 0.00 C 273 CD1 LEU A 23141.223 -3.993 8.628 1.00 0.00 C **ATOM** 274 CD2 LEU A 23143.478 -3.780 7.569 1.00 0.00 C ATOM 275 H LEUA 23140.533 -0.463 7.189 1.00 0.00 H **ATOM ATOM** 276 HA LEUA 23142.940 -1.353 5.819 1.00 0.00 H 277 1HB LEU A 23140.400 -2.790 6.586 1.00 0.00 H **ATOM** 278 2HB LEU A 23141.738 -3.549 5.744 1.00 0.00 H **ATOM** 279 HG LEU A 23142.300 -2.191 8.337 1.00 0.00 H **ATOM** 280 1HD1 LEU A 23140.326 -3.448 8.885 1.00 0.00 H **ATOM** 281 2HD1 LEU A 23141.738 -4.284 9.532 1.00 0.00 H **ATOM** 282 3HD1 LEU A 23140.960 -4.875 8.064 1.00 0.00 H ATOM 283 1HD2 LEU A 23144.046 -3.218 6.842 1.00 0.00 H ATOM 284 2HD2 LEU A 23143.323 -4.785 7.206 1.00 0.00 H **ATOM** 285 3HD2 LEU A 23144.021 -3.815 8.502 1.00 0.00 H ATOM 286 N ALAA 24142.088 -1.802 3.466 1.00 0.00 N **ATOM** 287 CA ALAA 24141.682 -1.753 2.067 1.00 0.00 C ATOM ATOM 288 C ALA A 24142.361 -2.855 1.260 1.00 0.00 C

ATOM 289 O ALAA 24143.394 -3.389 1.666 1.00 0.00 O **ATOM** 290 CB ALAA 24142.002 -0.390 1.473 1.00 0.00 C 291 H ALAA 24142.947 -2.210 3.702 1.00 0.00 H **ATOM** 292 HA ALA A 24140.613 -1.896 2.025 1.00 0.00 H **ATOM** 293 1HB ALAA 24142.207 -0.495 0.418 1.00 0.00 H ATOM 294 2HB ALA A 24142.867 0.025 1.969 1.00 0.00 H ATOM 295 3HB ALAA 24141.158 0.270 1.612 1.00 0.00 H **ATOM** 296 N GLUA 25141.774 -3.190 0.116 1.00 0.00 N **ATOM** 297 CA GLU A 25142.323 -4.228 -0.749 1.00 0.00 C **ATOM** 298 C GLUA 25142.602 -3.682 -2.145 1.00 0.00 C **ATOM** 299 O GLUA 25141.870 -2.827 -2.646 1.00 0.00 O **ATOM** 300 CB GLU A 25141.356 -5.412 -0.836 1.00 0.00 C **ATOM** 301 CG GLU A 25142.003 -6.689 -1.347 1.00 0.00 C **ATOM** 302 CD GLU A 25141.070 -7.505 -2.220 1.00 0.00 C **ATOM** 303 OE1 GLU A 25141.035 -8.742 -2.056 1.00 0.00 O **ATOM ATOM** 304 OE2 GLU A 25140.376 -6.906 -3.068 1.00 0.00 O 305 H GLUA 25140.954 -2.728 -0.154 1.00 0.00 H **ATOM** 306 HA GLU A 25143.252 -4.566 -0.315 1.00 0.00 H **ATOM** 307 1HB GLU A 25140.955 -5.606 0.147 1.00 0.00 H **ATOM ATOM** 308 2HB GLU A 25140.547 -5.152 -1.501 1.00 0.00 H **ATOM** 309 1HG GLUA 25142.877 -6.428 -1.926 1.00 0.00 H 310 2HG GLU A 25142.299 -7.291 -0.501 1.00 0.00 H **ATOM ATOM** 311 N VALA 26143.665 -4.180 -2.768 1.00 0.00 N 312 CA VALA 26144.042 -3.740 -4.107 1.00 0.00 C ATOM 313 C VALA 26143.862 -4.863 -5.123 1.00 0.00 C **ATOM** 314 O VALA 26144.363 -5.971 -4.934 1.00 0.00 O **ATOM** 315 CB VALA 26145.503 -3.253 -4.149 1.00 0.00 C **ATOM** 316 CG1 VAL A 26145.828 -2.646 -5.506 1.00 0.00 C ATOM 317 CG2 VAL A 26145.767 -2.253 -3.033 1.00 0.00 C ATOM 318 H VALA 26144.210 -4.857 -2.317 1.00 0.00 H ATOM 319 HA VALA 26143.400 -2.915 -4.380 1.00 0.00 H ATOM

ATOM